COMPUTATIONAL NUCLEAR PHYSICS
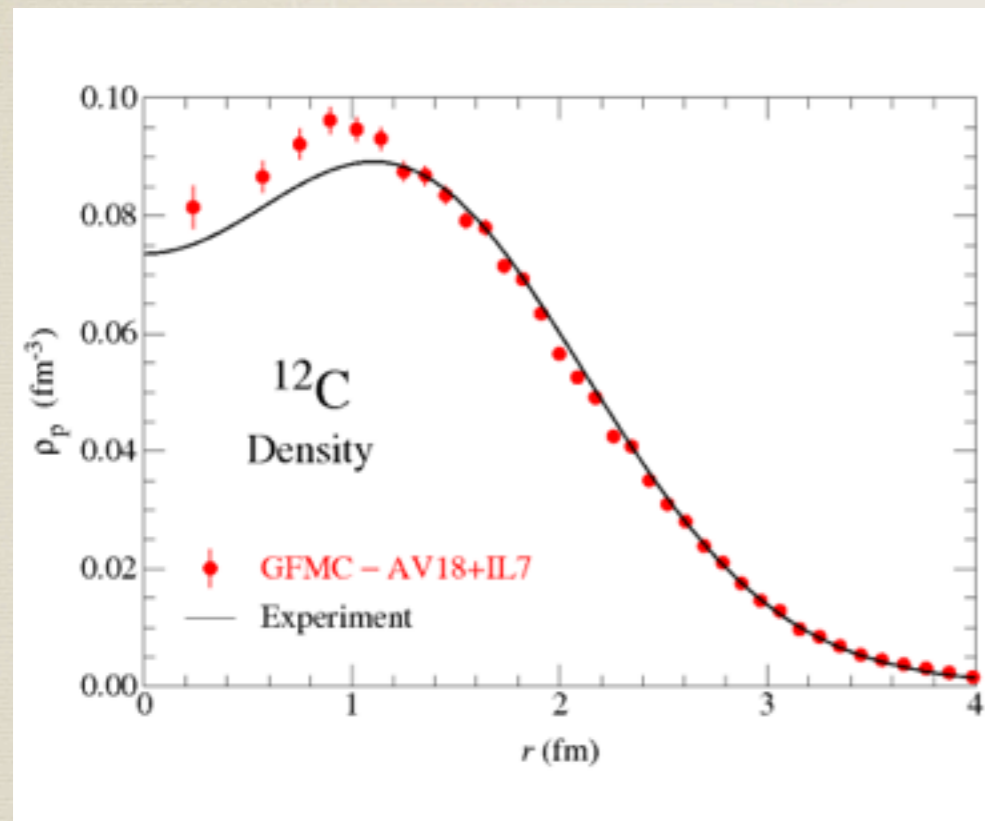
Kostas Orginos

Jefferson Lab
Thomas Jefferson National Accelerator Facility

We study nuclear physics using the worlds largest computers

Computational Physics: Probe the fundamental theory by performing virtual experiments

Computational Nuclear Physics

^{12}C Density

GFMC − AV18+IL7

Experiment

UNEDF collaboration
http://www.unedf.org

* Parametrize the nucleon-nucleon potential

  * AV18: 40 adjustable parameters

* Fit to low energy nucleon-nucleon scattering data

  * AV18: 4301 nn, np scattering data with p<350MeV Phys. Rev. C 51, 38 (1995)

* Solve the many-body problem

  * GFMC, DFT, etc.

^{12}C binding energy: 93.5(6) MeV,
    Experiment: 92.16 MeV

Computational Nuclear Physics

^{12}C binding energy
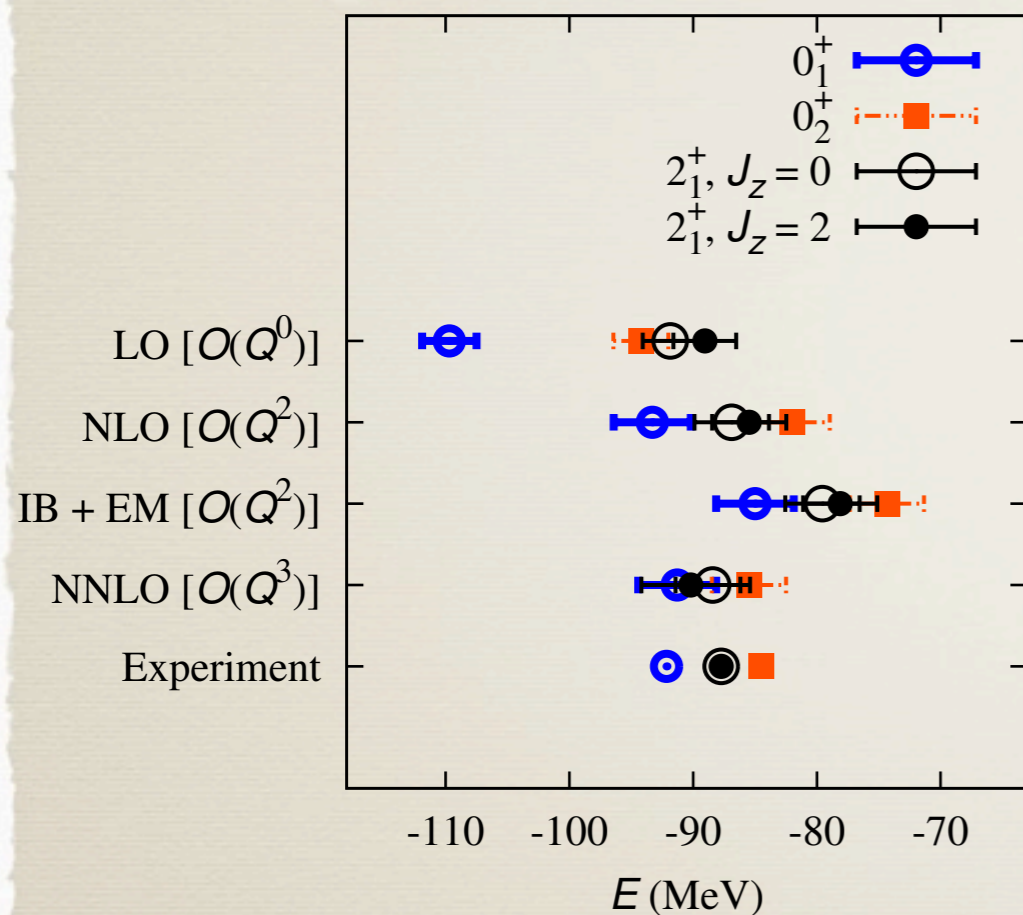
* Use chiral effective theory

  * Systematic expansion in momentum p and pion mass m_π

  * Includes chiral symmetry

  * Unknown low energy constants

* Fit the unknown low energy constants to low energy nucleon-nucleon scattering data

* Put the EFT on a lattice and solve using Quantum Monte Carlo (QMC)

Epelbaum *et al.* Eur.Phys.J. A45 (2010) 335
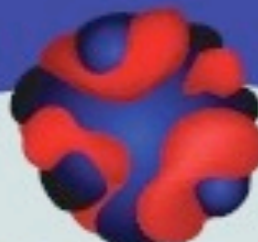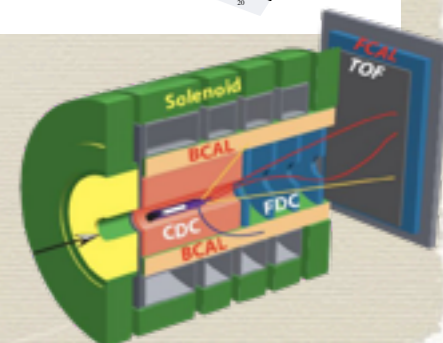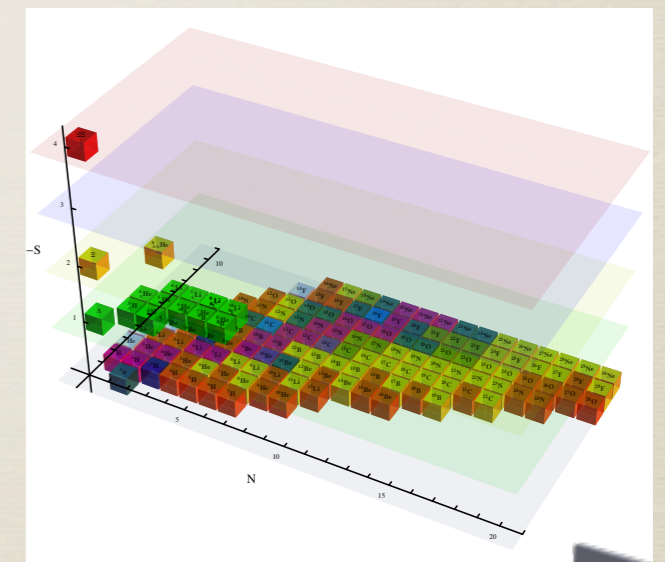
Figure by W. Nazarewicz

Hadron Interactions

Goals:

* Challenge: Compute properties of nuclei from QCD

  * Spectrum and structure

* Confirm well known experimental observation for two nucleon systems

* Explore the largely unknown territory of hyper-nuclear physics

* Provide input for the equation of state for nuclear matter in neutron stars

* Provide input for understanding the properties of multi-baryon systems

* Understand the spectrum of resonances in QCD

QCD: The theory

July 2009

$\alpha_s(Q)$

△ ▲ Deep Inelastic Scattering
○ ● e^+e^- Annihilation
□ ⊠ Heavy Quarkonia

▬▬ QCD $\alpha_s(M_Z) = 0.1184 \pm 0.0007$

Q [GeV]

Politzer, Gross, Wilczek 2004 Nobel prize
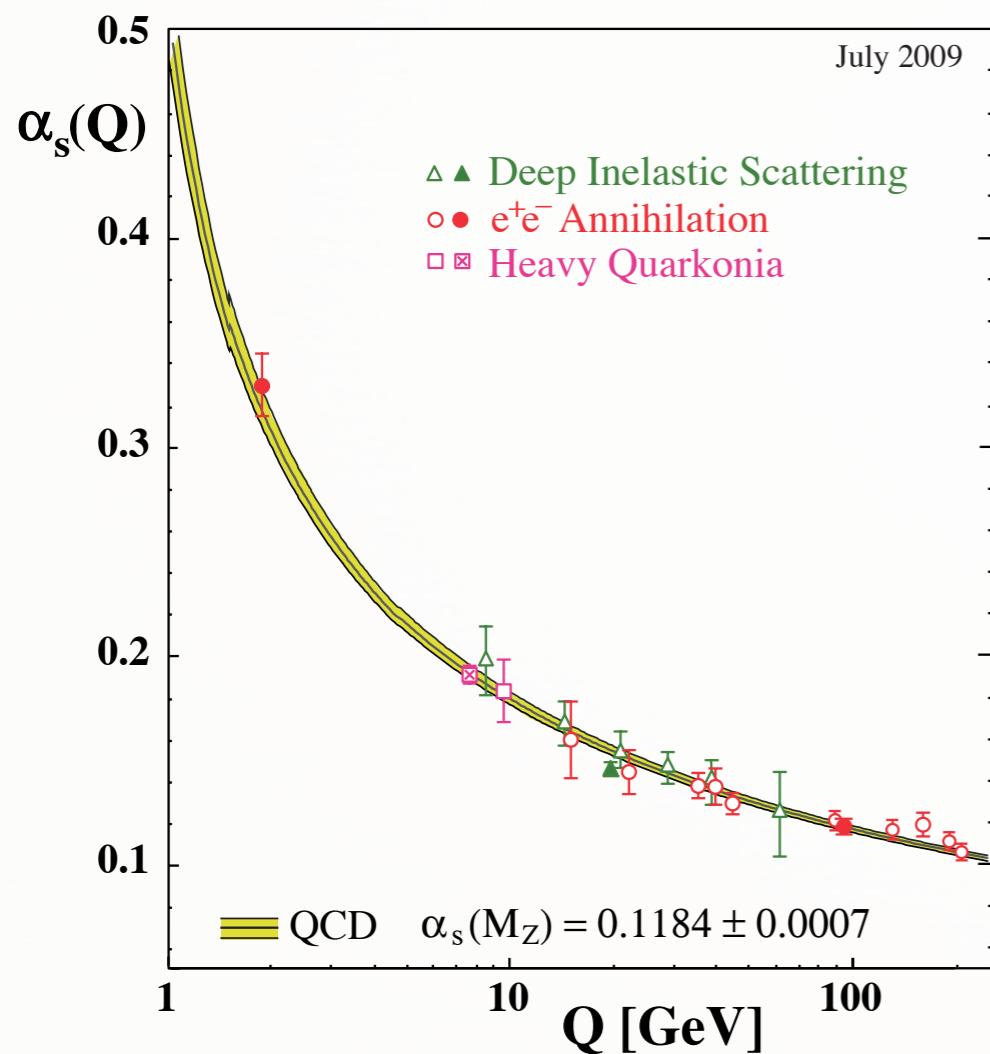
✳ Success of parton model

✳ Asymptotic Freedom:

  ✳ Interaction becomes weak at short distances

✳ Characteristic scale arises Λ_{qcd}

✳ Hadron masses:
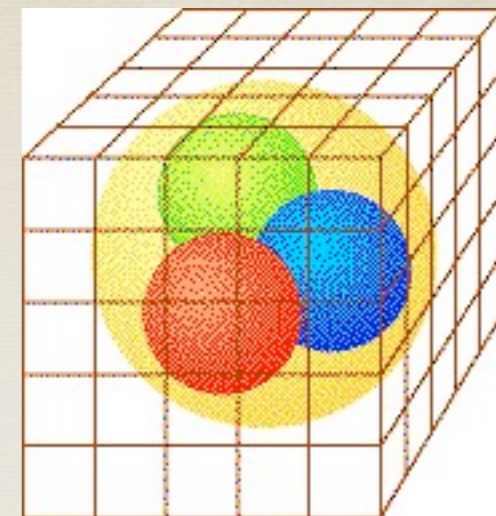
$$m = A \; \Lambda_{qcd}$$

✳ Quantum ChromoDynamics

QCD

Formulation

Path Integral

On a Lattice
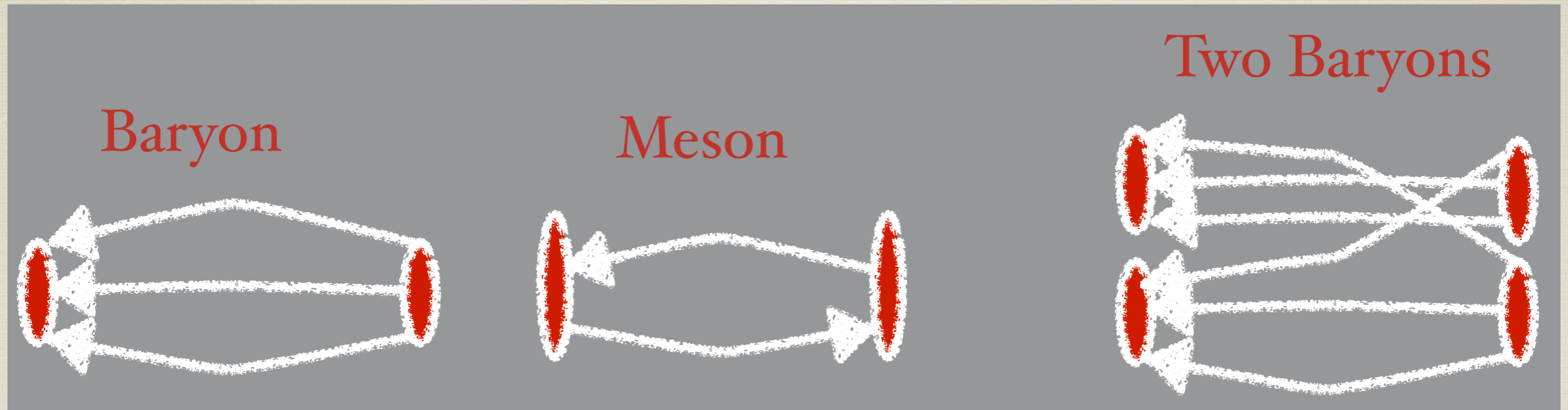
$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu,x} dU_\mu(x) \; \mathcal{O}[U, D(U)^{-1}] \; \det\left(D(U)^\dagger D(U)\right)^{n_f/2} \; e^{-S_g(U)}$$

Numerical calculations:

* Euclidean Lattice

* Ensemble of Gauge field configurations U

* Correlation function calculation as statistical averages

* Physical observables emerge in the continuum limit

Spectrum Calculations

Baryon

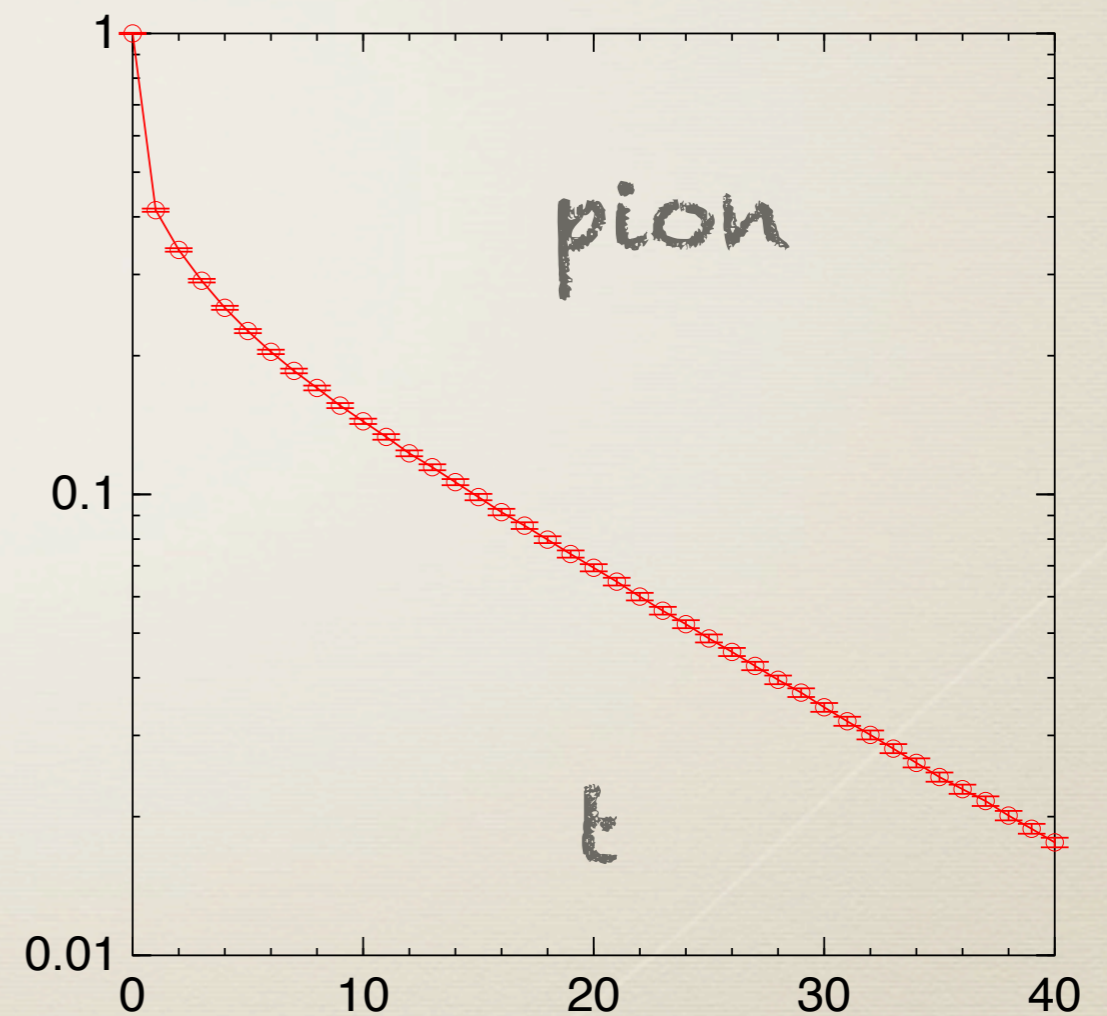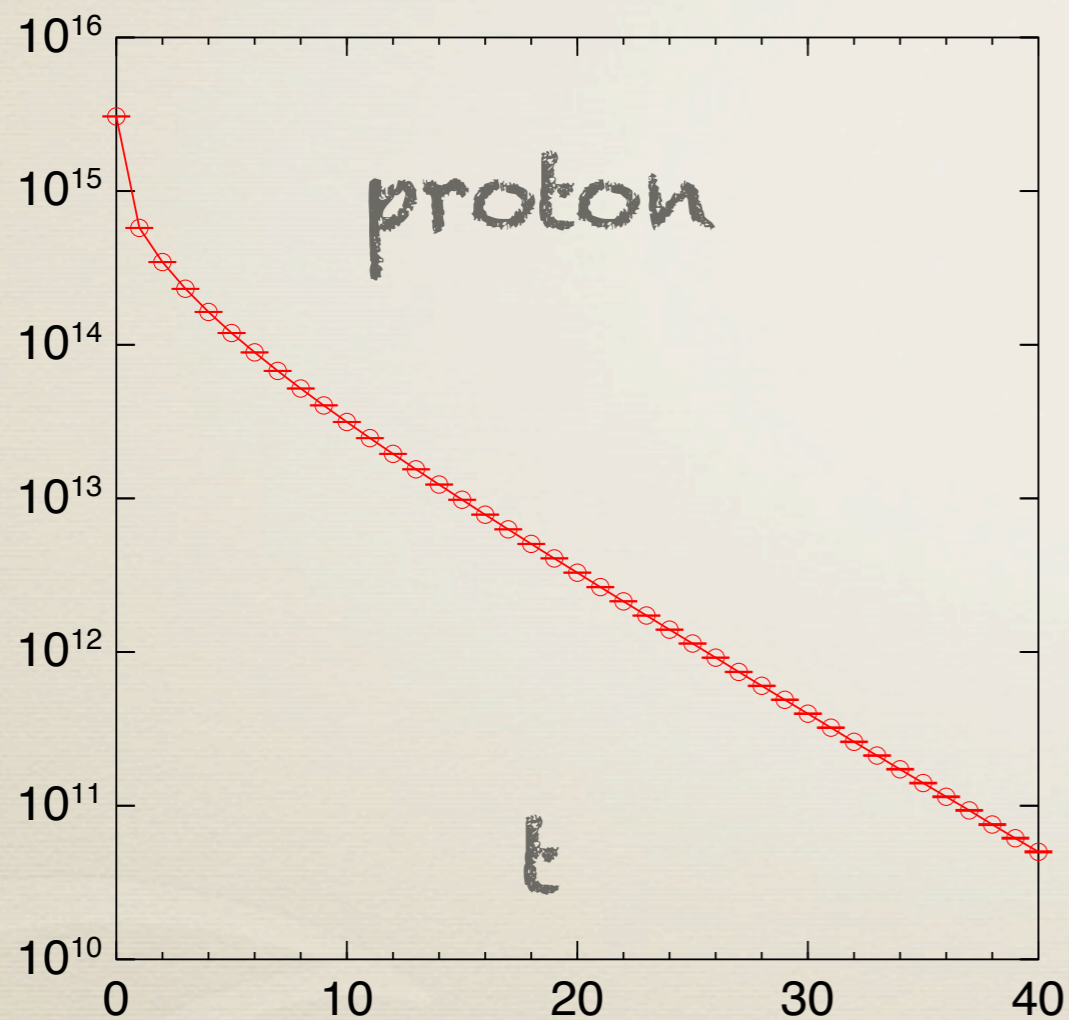Meson

Two Baryons

Lines in correspond to quark propagators

$$\langle q(x)\bar{q}(y) \rangle = D^{-1}(U)\big|_{x,y}$$

This computation dominates the calculation and makes it hard to compute with physical quark masses

Two point functions

$$C(t) \approx Z_0 e^{-m_0 t} + Z_1 e^{-m_1 t} + \cdots$$

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(U_i)$$

Scales of the problem

- Hadronic Scale: 1fm ~ 1×10^{-13} cm

- Lattice spacing << 1fm

  - take a=0.1fm

- Lattice size La >> 1fm

  - take La = 3fm

- Lattice 32^4

- Gauge degrees of freedom: $8 \times 4 \times 32^4 = 3.4 \times 10^7$
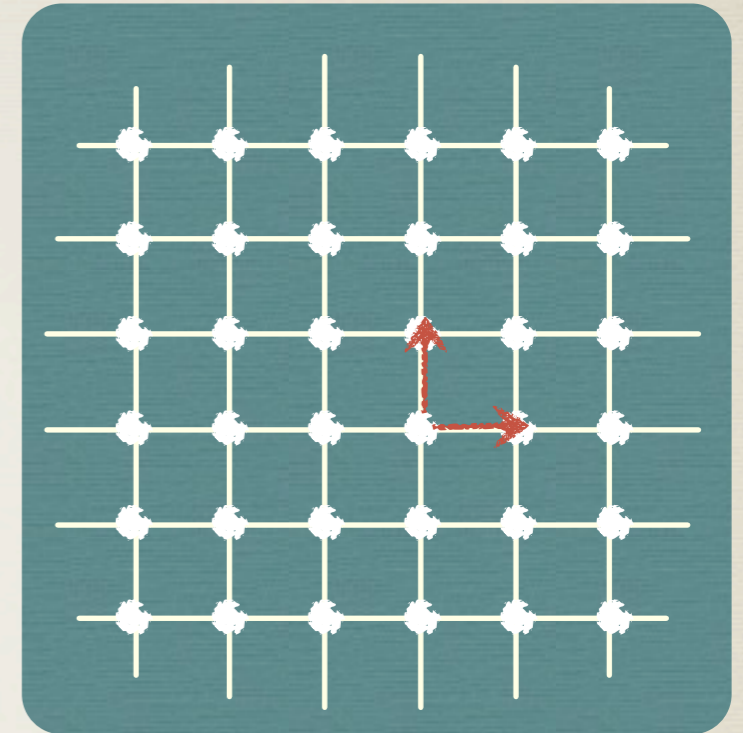
color

dimensions

sites

The pion mass is an
additional small scale

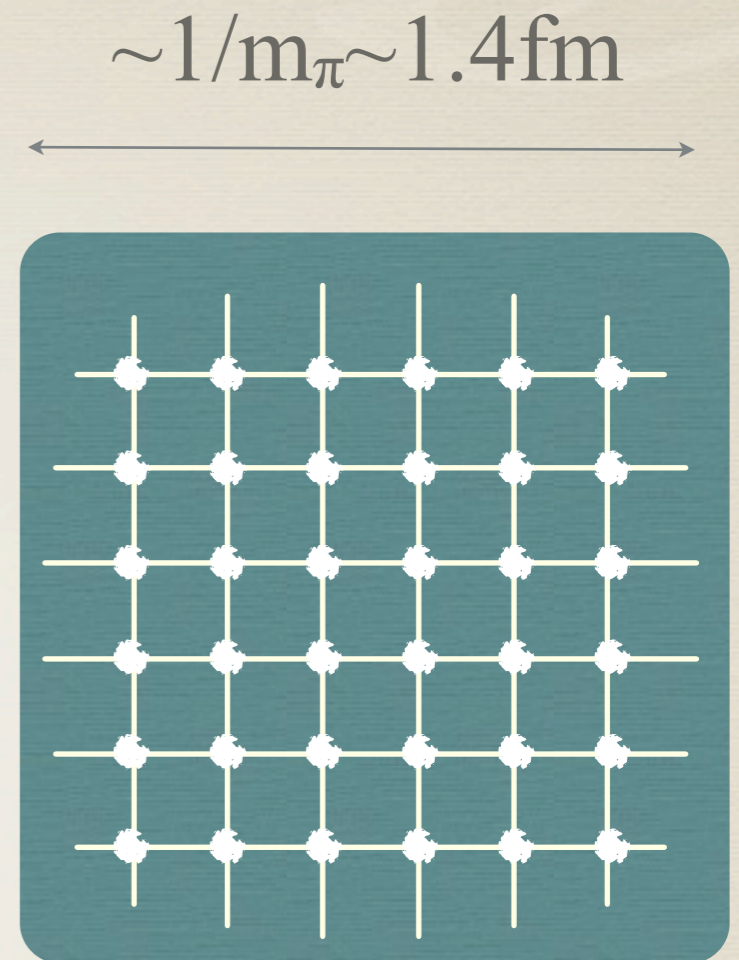Single hadron volume corrections

$$\sim e^{-m_\pi L}$$

~ 6 fm boxes are needed

Two hadron bound state volume
corrections $\sim e^{-\kappa L}$

Binding momentum κ of the deuteron ~ 45MeV

Nuclear energy level splittings are a few MeV

Box sizes of about 10 fm will be needed

Bound States

$$E_b = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2} - m_1 - m_2 \qquad p^2 < 0$$

$$E_b \approx \frac{p^2}{2\mu} = -\frac{\kappa^2}{2\mu} \qquad \kappa = |p|$$

κ is the "binding momentum" and μ the reduced mass

Finite volume corrections:

$$\Delta E_b = -3|A|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2}\kappa L}\right) \qquad \text{cubic group irrep: } A_1^+$$

Scattering on the Lattice

Elastic scattering amplitude (s-wave):

$$A(p) = \rangle\!\!\langle \;+\; \rangle\!\bigcirc\!\langle \;+\; \rangle\!\bigcirc\!\bigcirc\!\langle \;+\; \cdots$$

$$A(p) = \frac{4\pi}{m}\frac{1}{p\cot\delta - ip}$$

At finite volume one can show:

$$E_n = 2\sqrt{p_n^2 + m^2}$$

$$p\cot\delta(p) = \frac{1}{\pi L}\, \mathbf{S}\left(\frac{p^2 L^2}{4\pi^2}\right) \qquad\qquad \mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{|\mathbf{j}|<\Lambda}\frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda$$
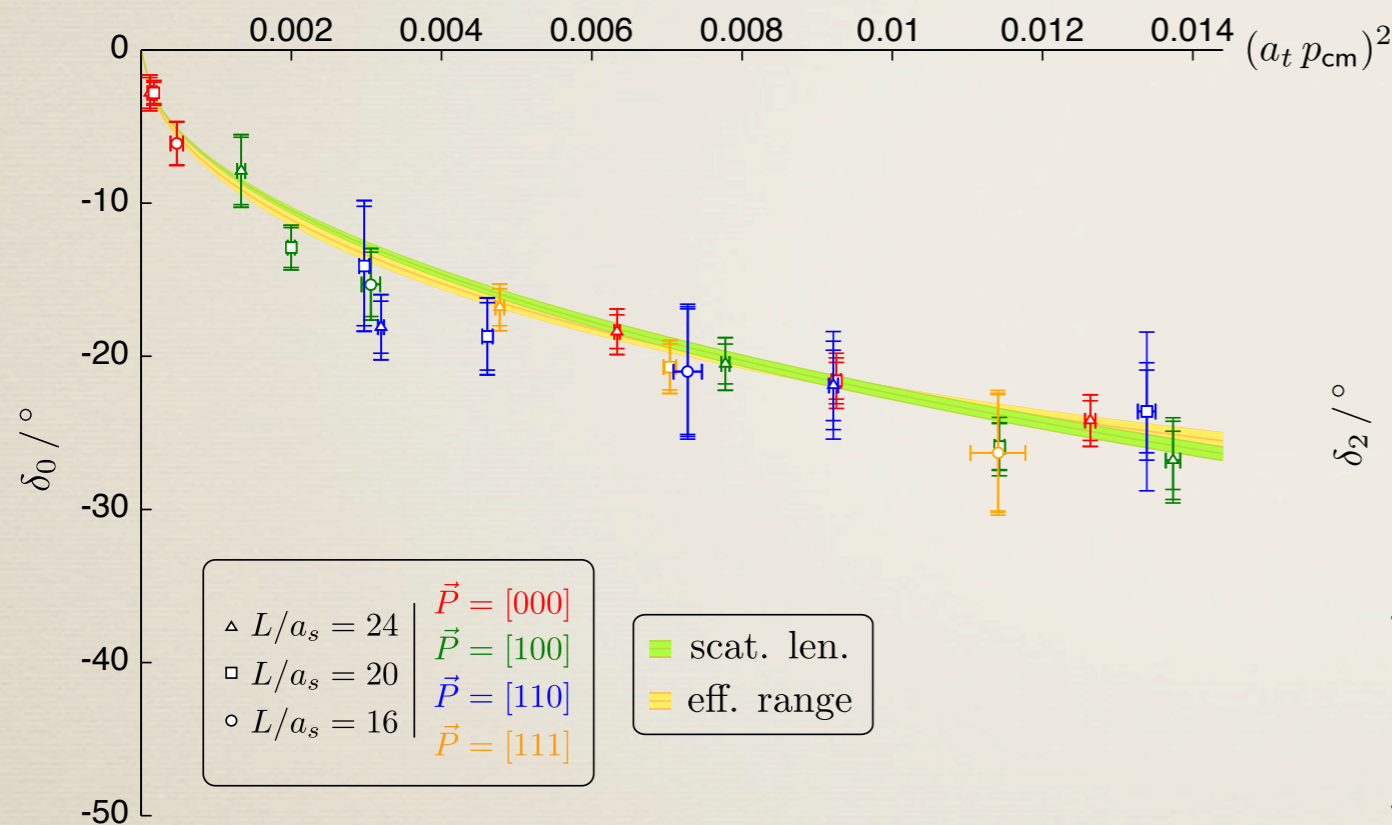
Small p:

$$p\cot\delta(p) = \frac{1}{a} + \frac{1}{2}rp^2 + \dots.$$
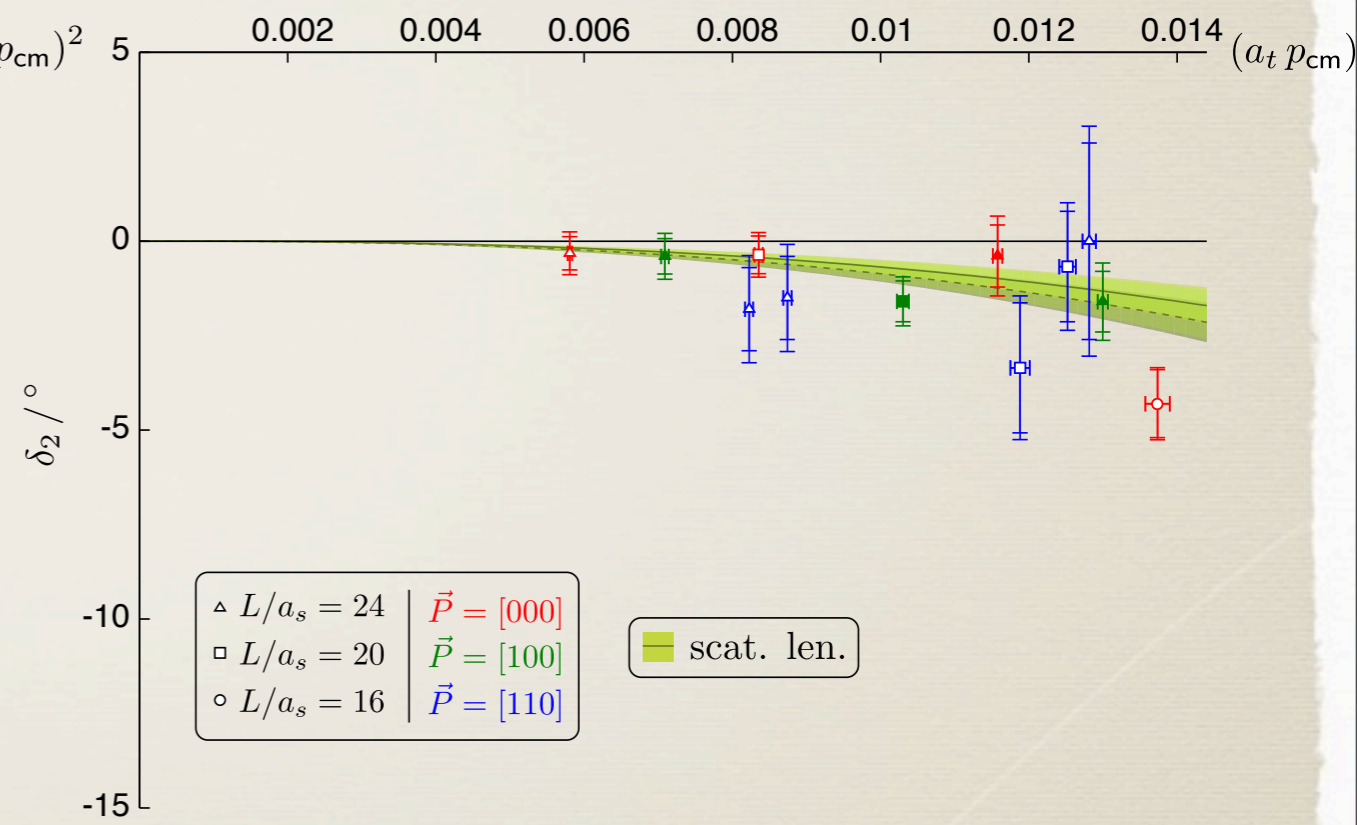
a is the scattering length

Phase shifts: π-π I=2

[J. Dudek *et al*. arXiv: 1203.6041]

Hadron Spectrum/JLAB

S-Wave

D-Wave

Two Nucleon spectrum
free nucleons

3fm box
24³ lattice

anisotropy factor 3.5

$M_\pi = 390\,MeV$

Two Nucleon spectrum

free 2 particle spectrum

$M_\pi = 390\,MeV$

M_n
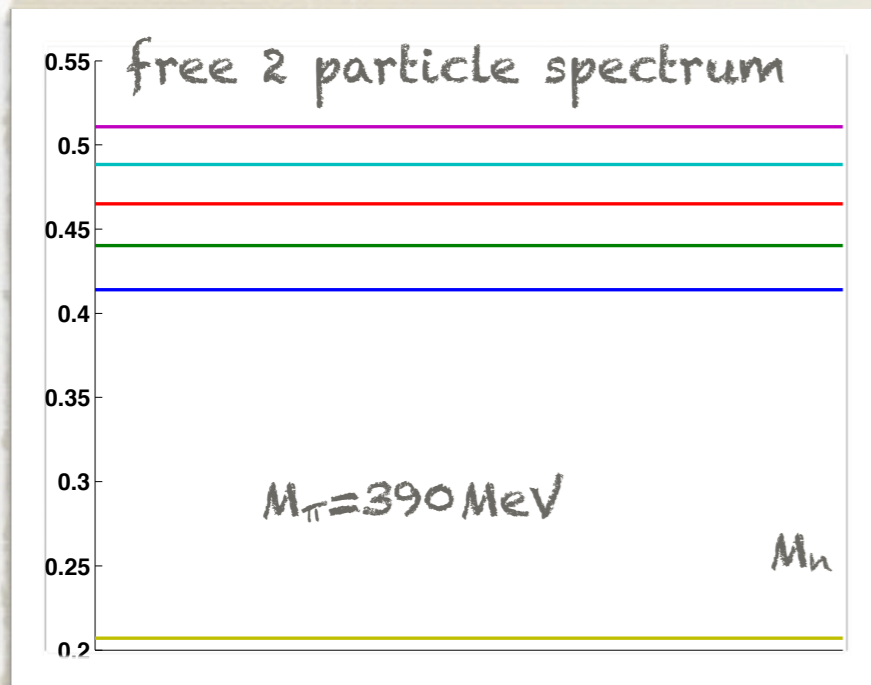
3fm box   24³ lattice

anisotropy factor 3.5

* Dense spectrum requires long requires precise determination of correlation functions are large Euclidean time separations

* However, the signal fades exponentially fast in the Euclidean time separation

Signal to Noise

$$StoN = \frac{C(t)}{\sqrt{var(C(t))}} =\sim Ae^{-(M_N - 3/2m_\pi)t}$$
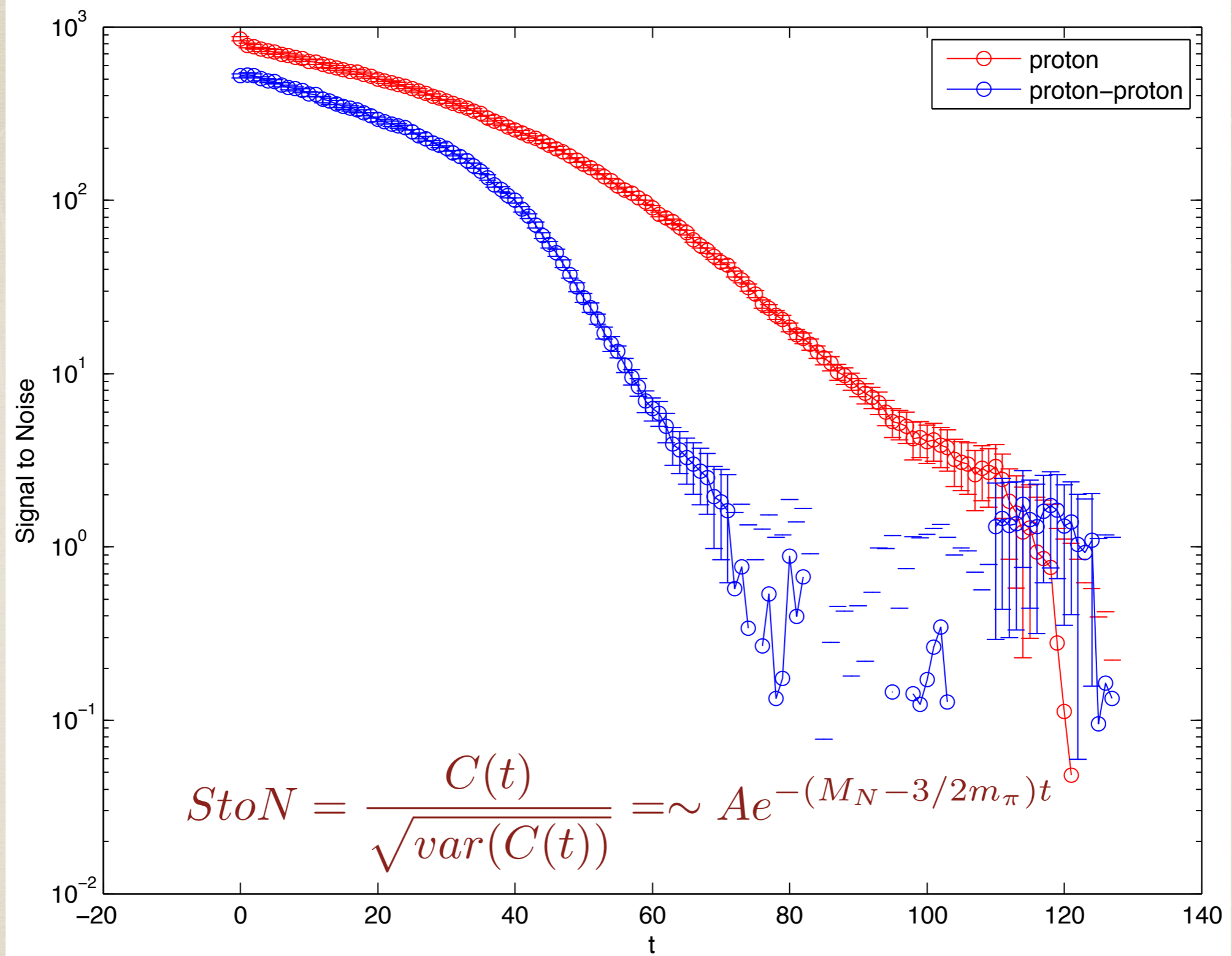
$32^3 \times 256$
$M_\pi = 390 \text{MeV}$

anisotropy factor 3.5

NPLQCD data

Wednesday, June 26, 13

Challenges

* New scales that are much smaller than characteristic QCD scale appear

* The spectrum is complicated and more difficult to extract from euclidean correlators

* Construction of multi-quark correlations functions may be computationally expensive

* Monte-Carlo evaluation of correlation functions converges slowly

Challenges

* New scales that are much smaller than characteristic QCD scale appear

* The spectrum is complicated and more difficult to extract from euclidean correlators

* Construction of multi-quark correlations functions may be computationally expensive

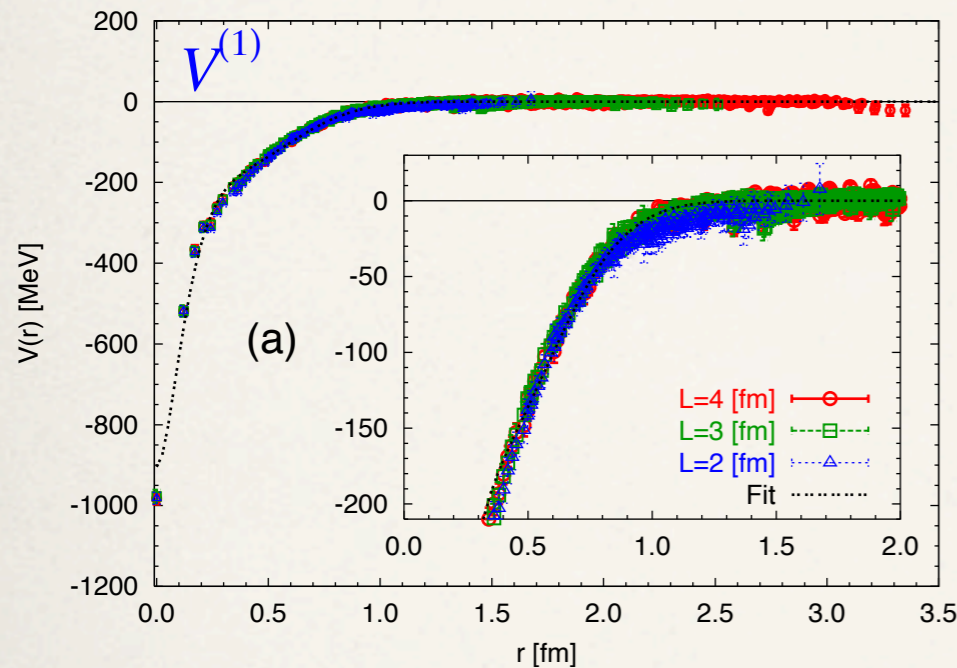* Monte-Carlo evaluation of correlation functions converges slowly
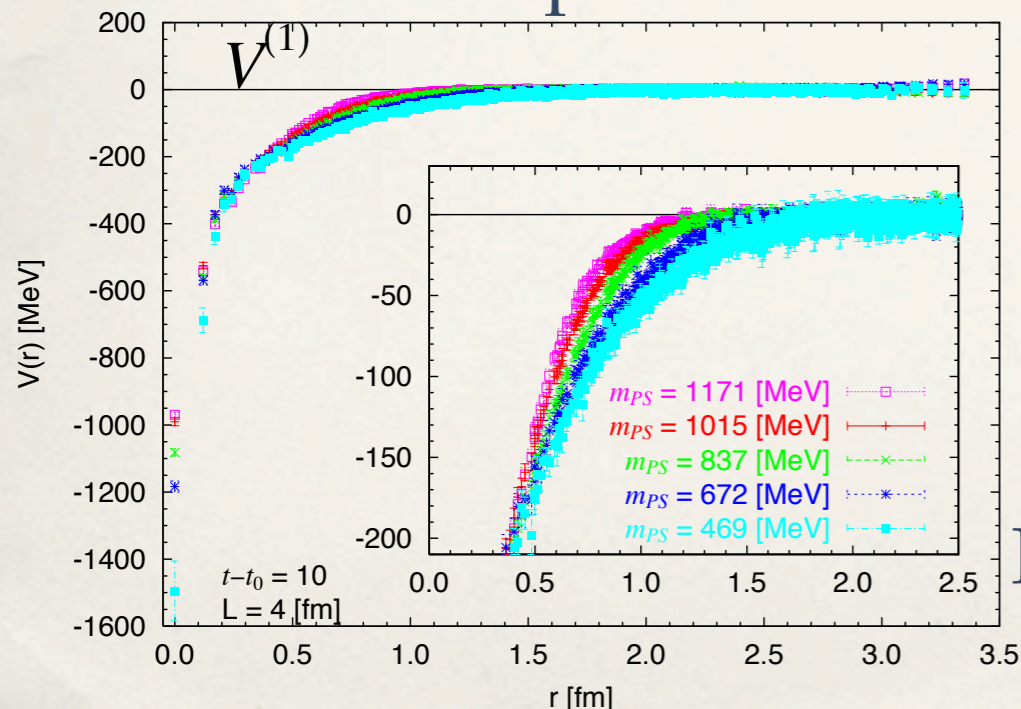
We really need better algorithms to deal with an exponentially hard problem

HALQCD

Volume dependence

Mass dependence

* Nambu-Bethe-Salpeter (NBS) wave function

$$\phi_n(\vec{r}) = \langle 0|(BB)^{(\alpha)}(\vec{r},0)|W_n;\alpha\rangle$$

* Time dependent NBS

$$H_0\phi_n(\vec{r},t) + \int d^3r' U(\vec{r},\vec{r}')\phi_n(\vec{r}',t) = -\frac{\partial}{\partial t}\phi_n(\vec{r},t)$$
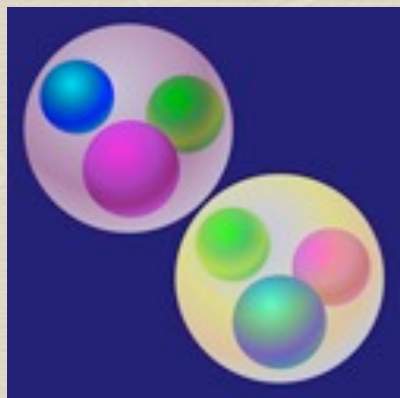
* Local potential approximation

$$V_C(r) = \frac{(\frac{\nabla^2}{2\mu} - \frac{\partial}{\partial t})\phi(\vec{r},t)}{\phi(\vec{r},t)}$$

Solve in infinite volume

$$\left(-\frac{\nabla^2}{2\mu} + V_C^f(r)\right)\psi(\vec{r},t) = -\frac{\partial}{\partial t}\psi(\vec{r},t)$$

Phase shifts and binding energies are computed

Wednesday, June 26, 13

H-dibaryon

R. L. Jaffe, Phys. Rev. Lett. 38, 195 (1977)

$S = -2,$
$B = 2,$
$J^P = 0^+$

* Proposed by R. Jaffe 1977

  * Perturbative color-spin interactions are attractive for (uuddss)

  * Diquark picture of scalar diquarks (ud)(ds)(su)

* Experimental searches of the H have not found it

  * BNL RHIC (+model): Excludes the region [-95, 0] MeV

    A. L. Trattner, PhD Thesis, LBL, UMI-32-54109 (2006).

  * KEK: Resonance near threshold

    C. J. Yoon et al., Phys. Rev. C 75, 022201 (2007).

* Several Lattice QCD calculations have been addressing the existence of a bound H

NPLQCD: lattice set up

* Anisotropic 2+1 clover fermion lattices

  * a ~ 0.125fm (anisotropy of ~ 3.5)

    Hadron Spectrum/JLAB

  * pion mass ~ 390 MeV

    * Volumes 16^3 x 128, 20^3 x 128, 24^3 x 128, 32^3 x 256

      largest box 4fm

    * Extrapolate to infinite volume using multiple volumes

$$\Delta E_b = -3|A|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2}\kappa L}\right)$$

  * Smeared source - 3 sink interpolating fields

  * second pion at 220 MeV

* Interpolating fields have the structure of s-wave Λ-Λ system

  * I=0, S=-2, A_1, positive parity
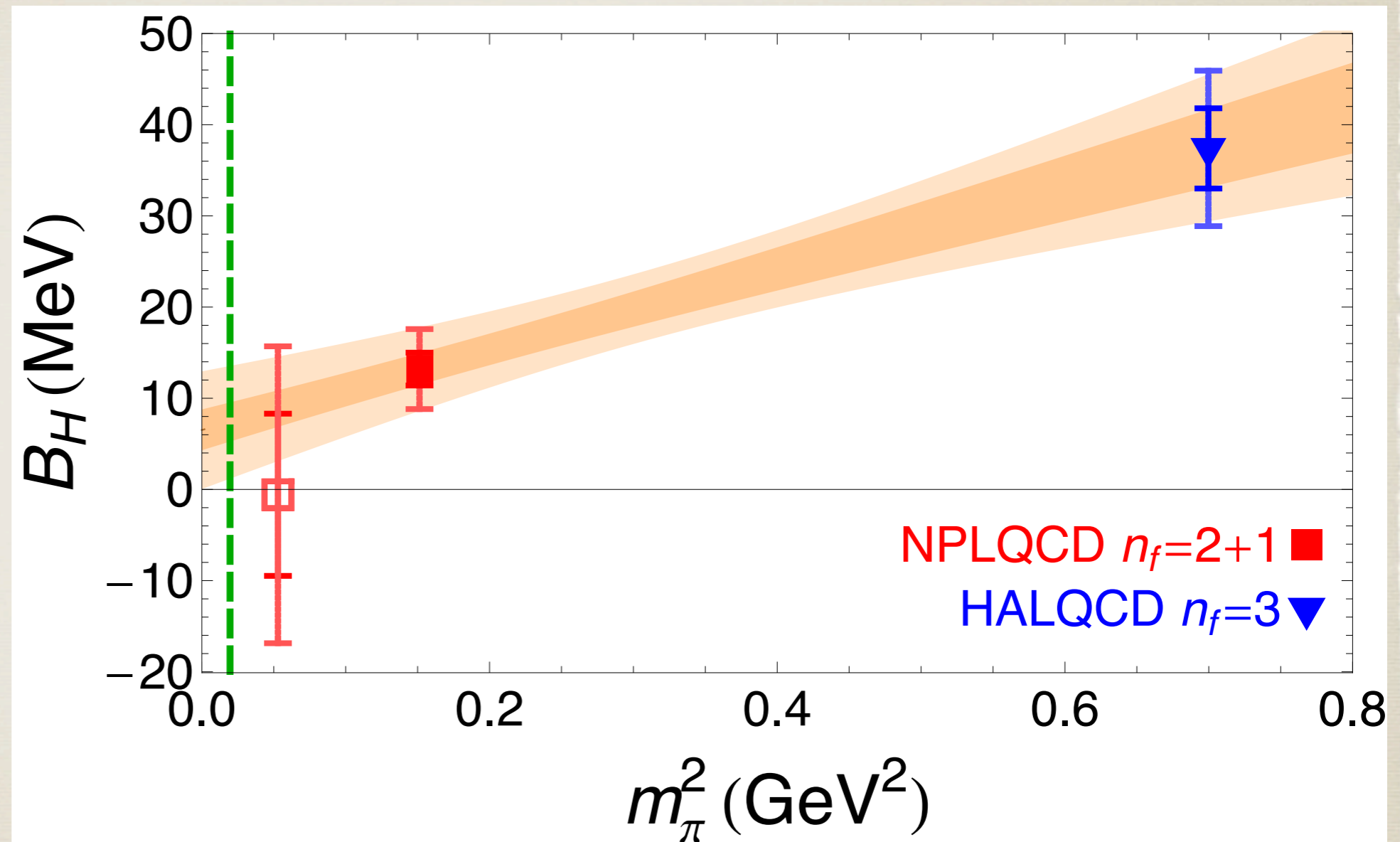
* Use very high statistics $O(500K)$ correlation functions

H-dibaryon: Towards the physical point

H-dibaryon:

Is bound at heavy
quark masses.
May be unbound at
the physical point

Continuum limit?
Isospin breaking?
Electromagnetism?

[S. Beane et.al. arXiv:1103.2821 Mod. Phys. Lett. A26: 2587, 2011]

HALQCD:Phys.Rev.Lett.106:162002,2011

ChiPT studies indicate the same trend:
P. Shanahan et.al. arXiv:1106.2851
J. Haidenbauer, Ulf-G. Meisner arXiv:1109.3590

NPLQCD

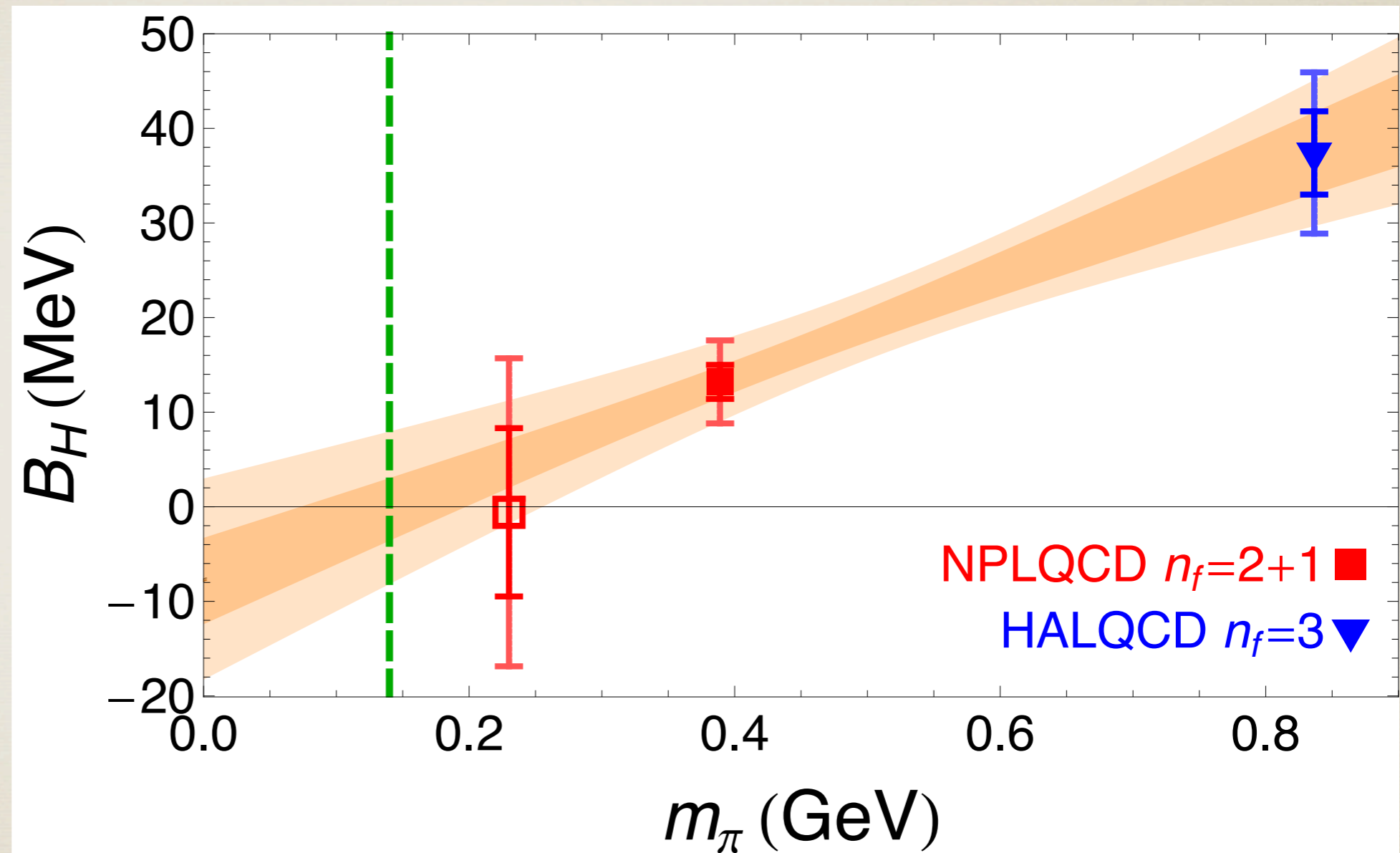# H-dibaryon: Towards the physical point

H-dibaryon:

Is bound at heavy
quark masses.
May be unbound at
the physical point

Continuum limit?
Isospin breaking?
Electromagnetism?

NPLQCD n_f=2+1 ■
HALQCD n_f=3 ▼

ChiPT studies indicate the same trend:

NPLQCD

Two baryon bound states

[S. Beane et.al. arXiv:1108.2889 Phys.Rev.D 85, 054511, 2012]
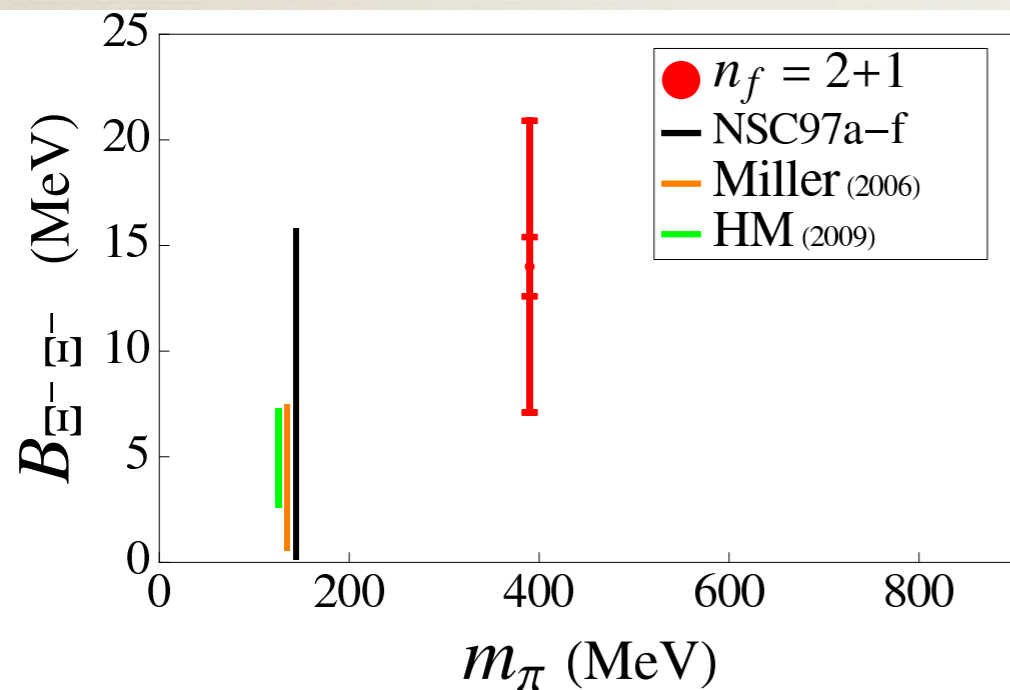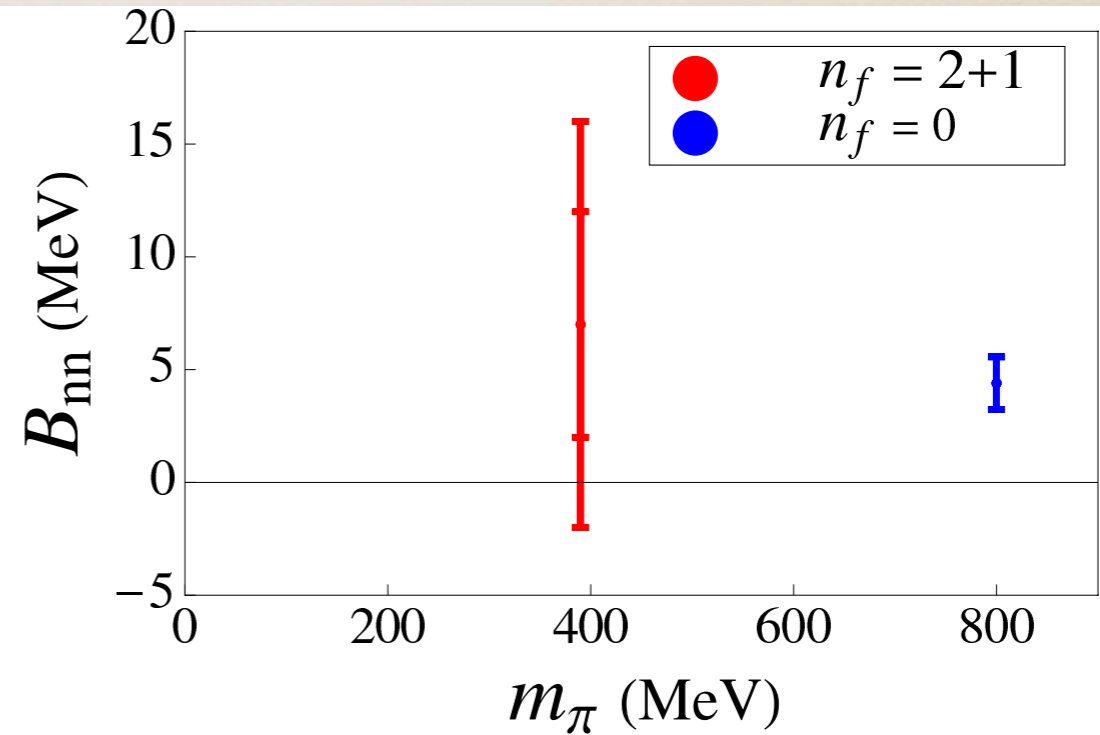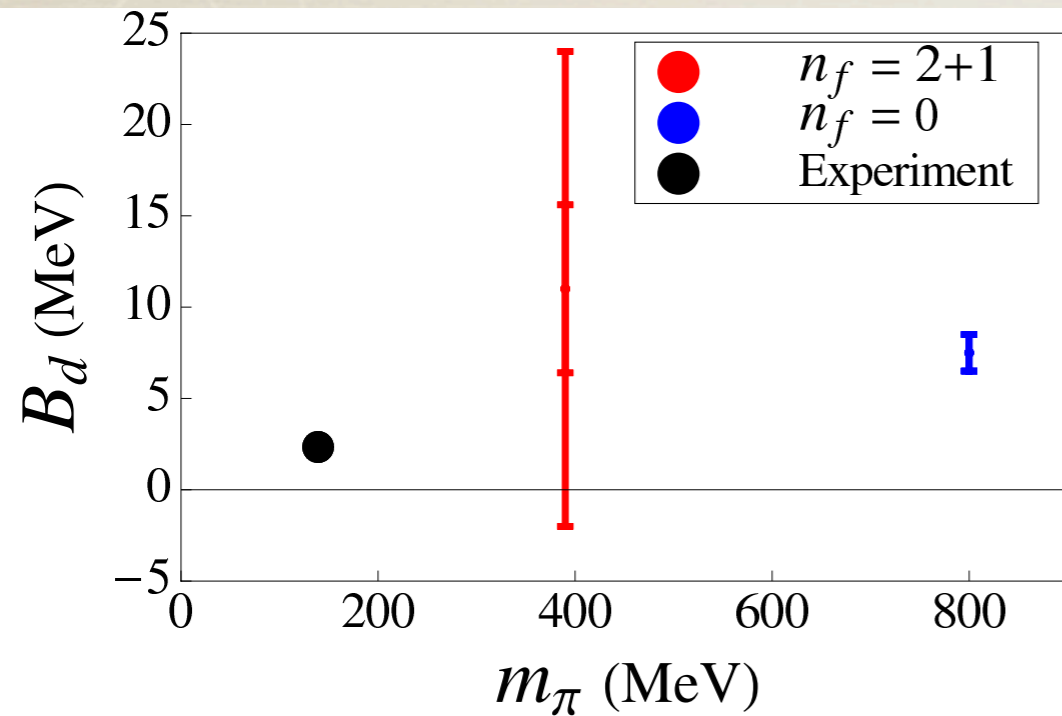
V. G. J. Stoks and T. A. Rijken
Phys. Rev. C 59, 3009 (1999)
[arXiv:nucl-th/9901028

G. A. Miller,
arXiv:nucl-th/0607006

J. Haidenbauer, Ulf-G. Meisner
Phys.Lett.B684,275-280(2010)
arXiv:0907.1395

n_f=0:
Yamazaki, Kuramashi, Ukawa
Phys.Rev. D84 (2011) 054506
arXiv: 1105.1418

gauge fields 2+1 flavors (JLab)
anisotropic clover $m_\pi \sim$ 390MeV

NPLQCD

Hyperon-Nucleon interactions
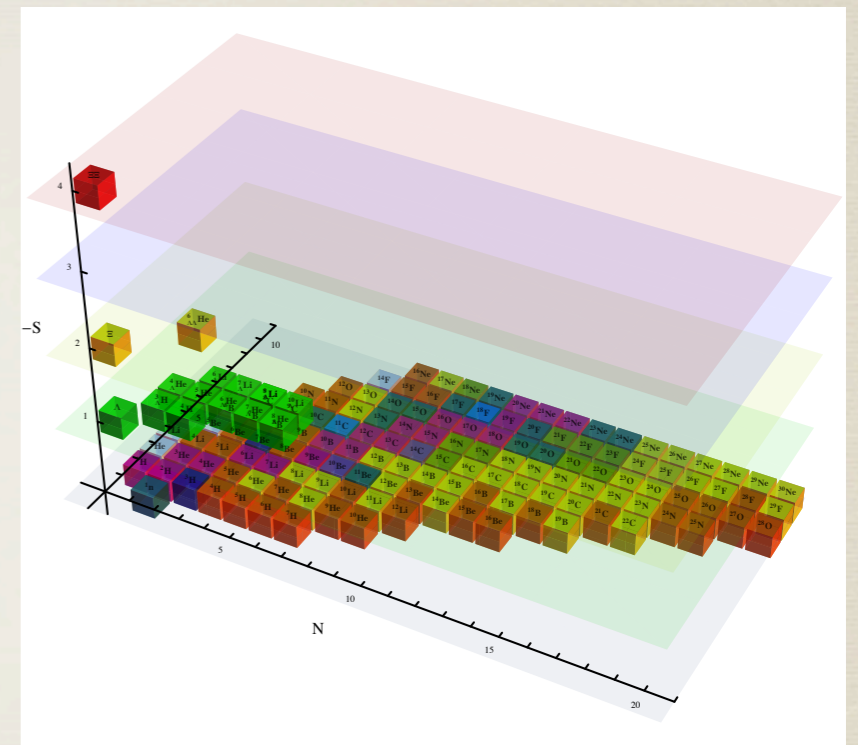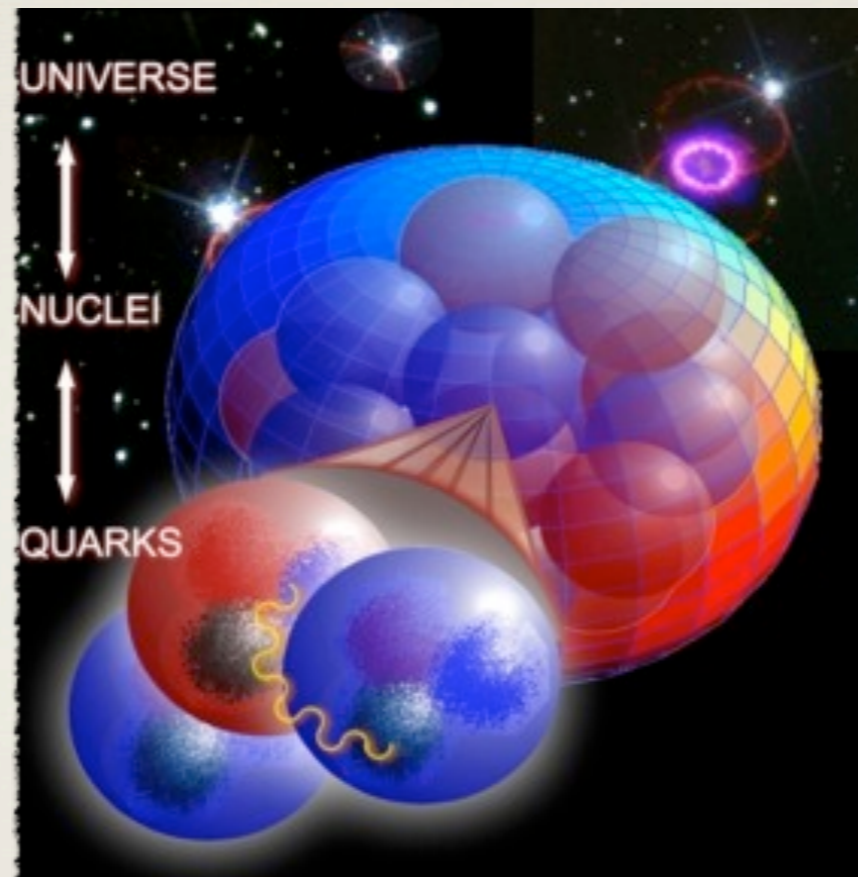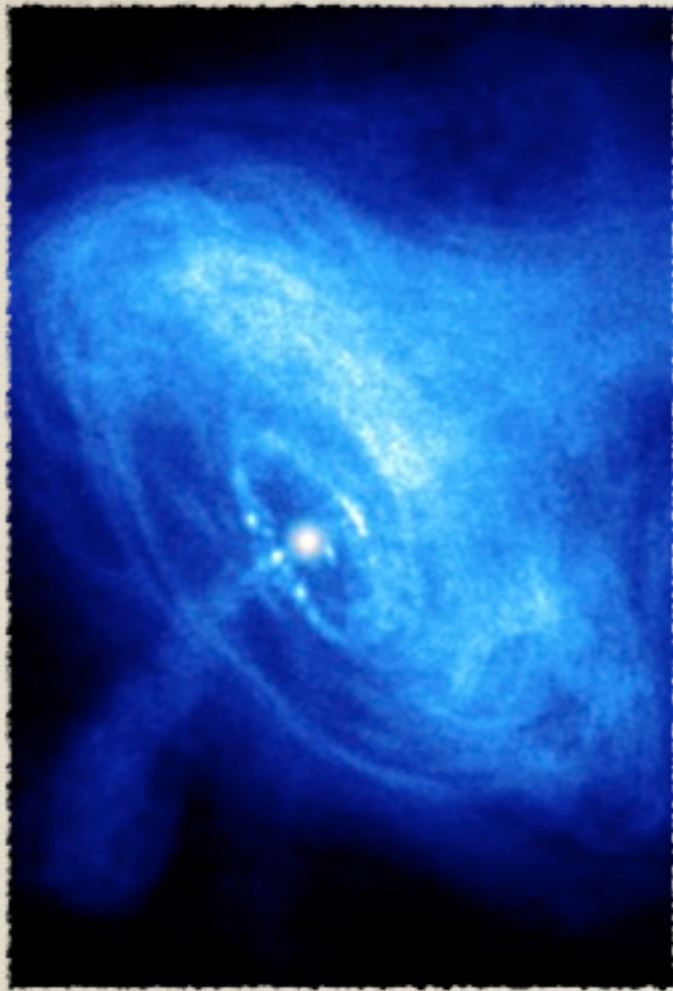
equation of state for nuclear matter in neutron stars

hyper-nuclear physics

Hyperon-Nucleon

[S. Beane et.al. arXiv:1204.3606 Phys. Rev. Lett. 109, 172001, 2012]
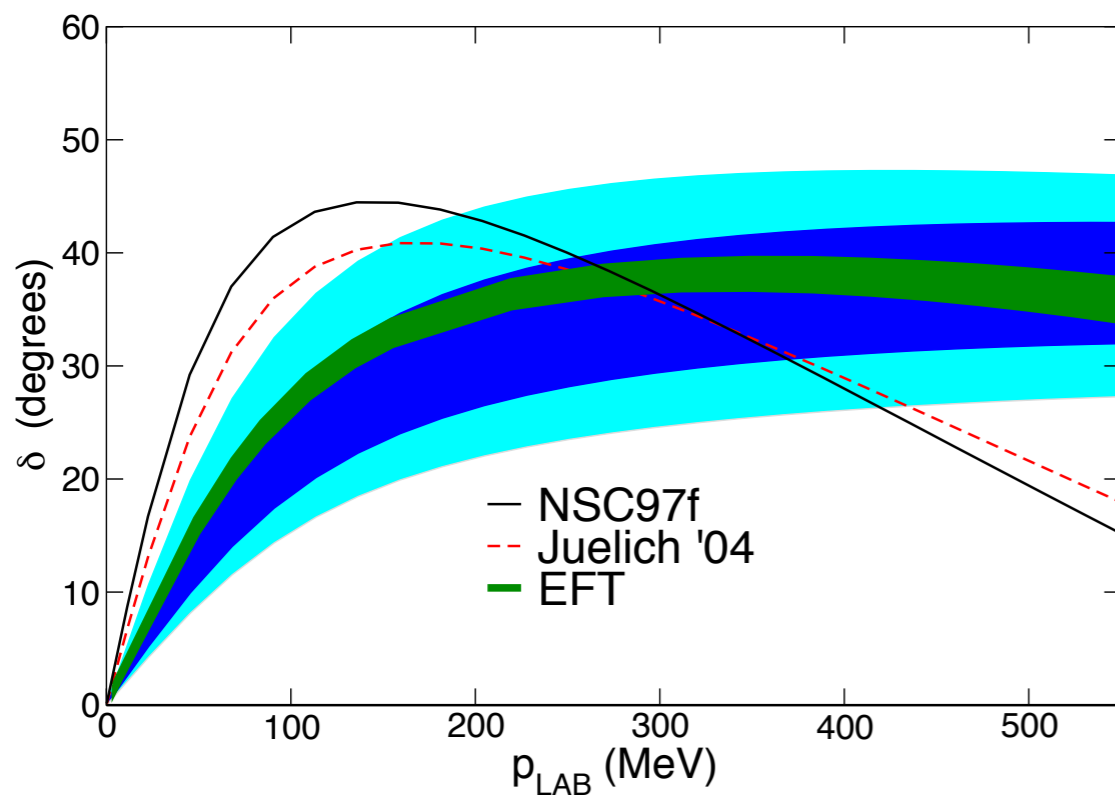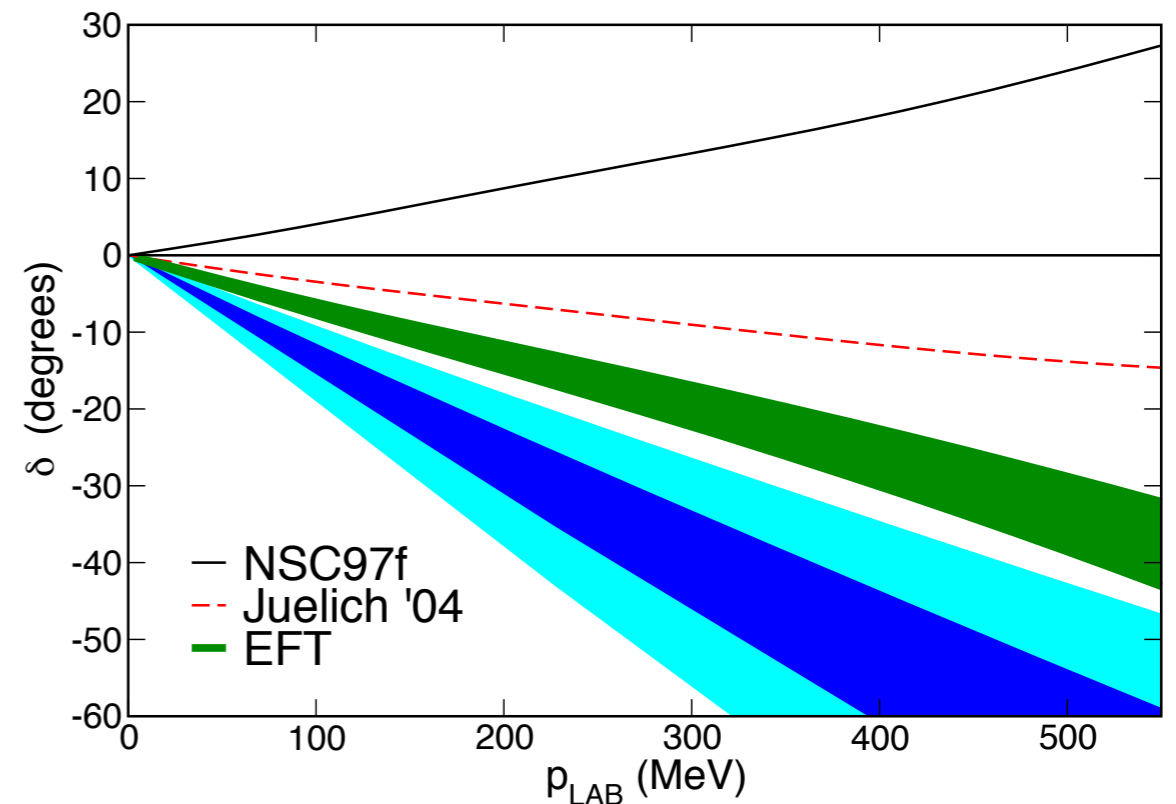
n-Σ spin singlet   n-Σ spin triplet

Lattice results constrain LO YN EFT

gauge fields 2+1 flavors (JLab) anisotropic clover $m_\pi \sim$ 390MeV   NPLQCD

Avoiding the noise

Work with heavy quarks

where the nucleon to pion mass gap becomes smaller

$$StoN = \frac{C(t)}{\sqrt{var(C(t))}} =\sim Ae^{-(M_N - 3/2m_\pi)t}$$

Lattice Setup

* Isotropic Clover Wilson with LW gauge action

  * Stout smeared (1-level)

  * Tadpole improved

* SU(3) symmetric point

  * Defined using m_π/m_Ω NPLQCD arXiv:1206.5219

* Lattice spacing 0.145 fm

                                                6000 configurations,

  * Set using Y spectroscopy   200 correlation functions per configuration

* Large volumes

  * 24^3 x 48 32^3 x 48 48^3 x 64

  * 3.5 fm   4.5 fm   7.0 fm

                                                computer time: XSEDE/NERSC

Nuclear spectrum
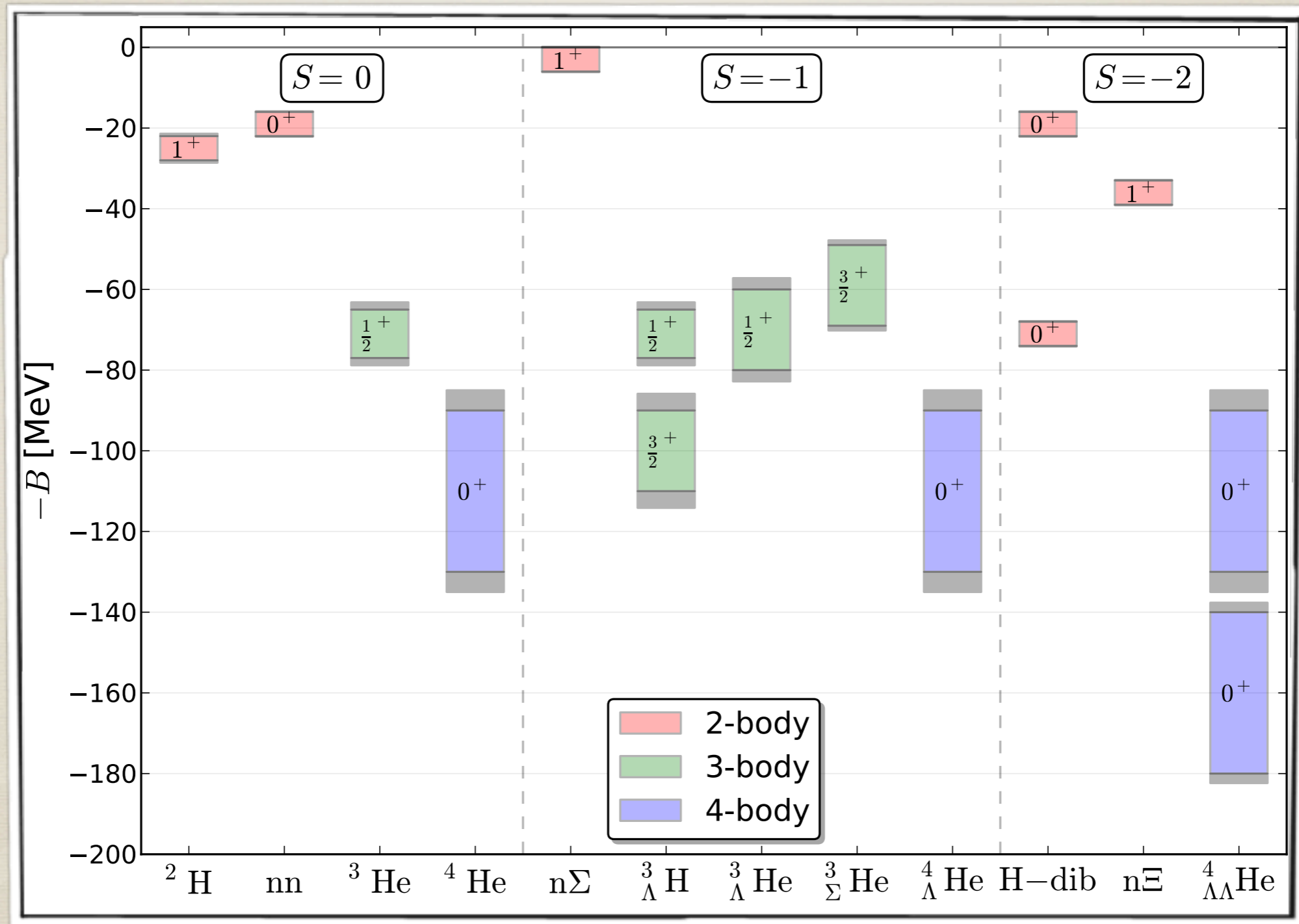
The deuteron

binding momentum
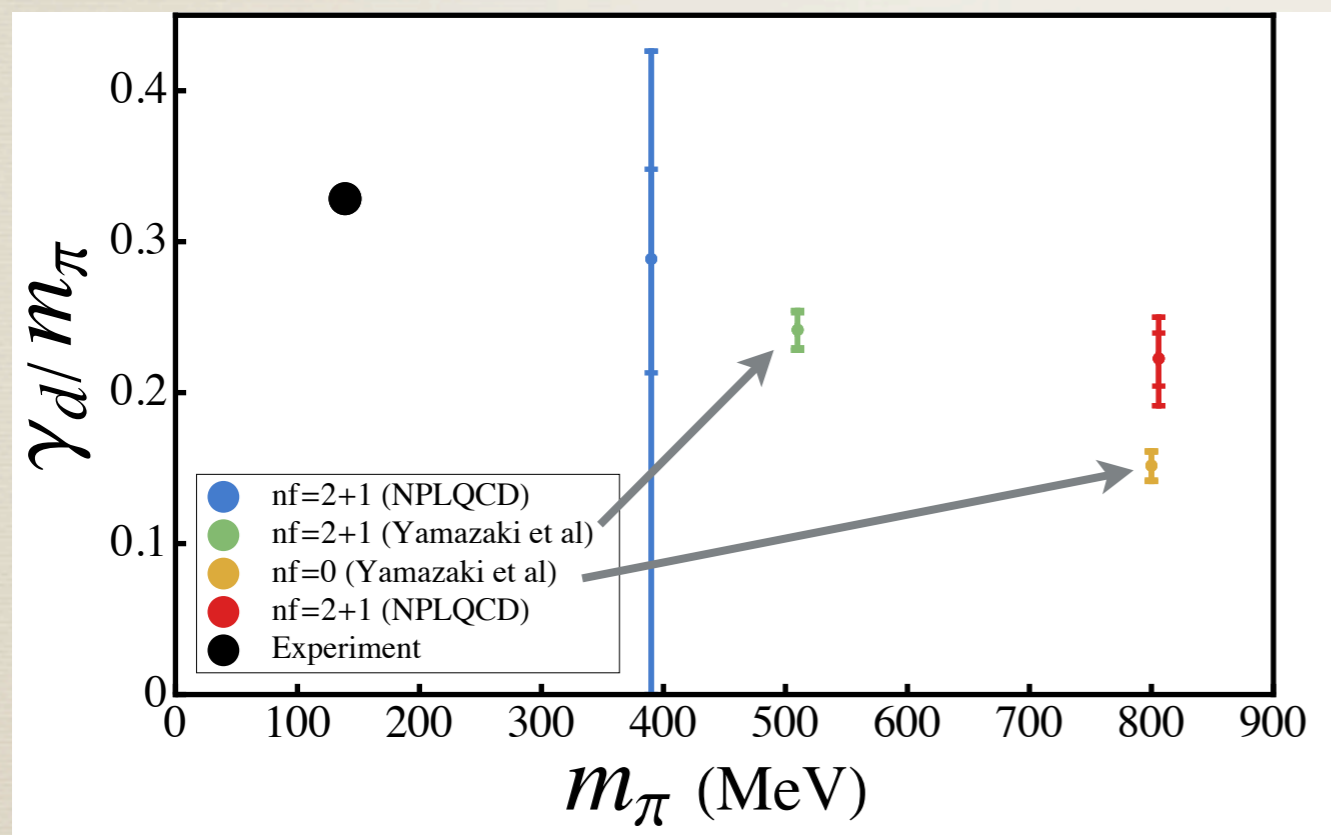
binding energy
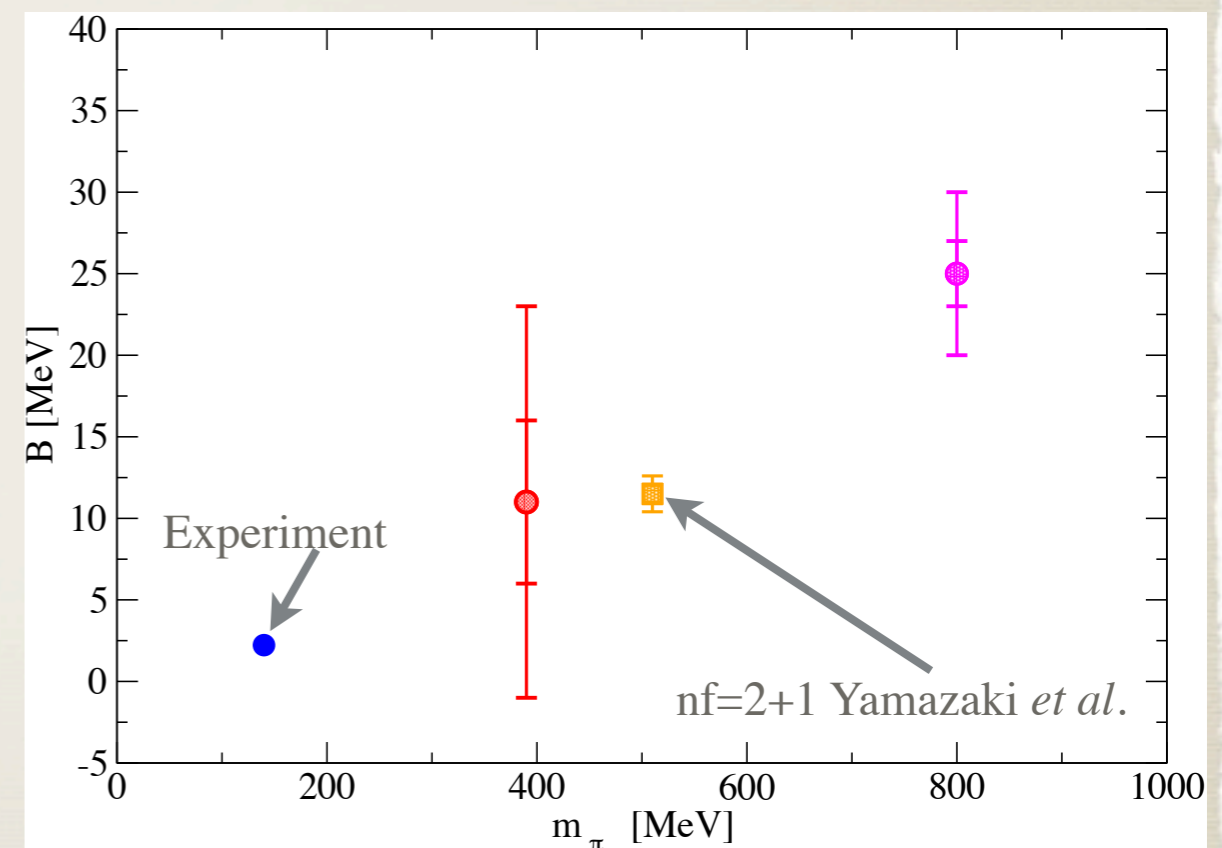
Lattice results seem consistent

The binding momentum seems to not vary much between the strange quark mass and the physical point in units of the pion mass

Nucleon Phase shifts

Elastic scattering amplitude (s-wave):

$$A(p) = \rightX + \rightXX + \rightXXX + \cdots$$

$$A(p) = \frac{4\pi}{m} \frac{1}{p \cot \delta - i p}$$

At finite volume one can show:

$$E_n = 2\sqrt{p_n^2 + m^2}$$

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S}\left(\frac{p^2 L^2}{4\pi^2}\right)$$

$$\mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{|\mathbf{j}| < \Lambda} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda$$

Small p:

$$p \cot \delta(p) = \frac{1}{a} + \frac{1}{2} r p^2 + \ldots$$

a is the scattering length

$$E(p) = 2\sqrt{p^2 + m^2} - 2m$$

Two Body spectrum in a box

$$p \cot\delta(p) = S\left(\frac{p^2 L^2}{4\pi^2}\right)$$

$$p \cot\delta(p) = \frac{1}{a} + r^2 p^2 + \cdots$$

E(p)

O

E₋₁

↑ k

↓ k

single point source
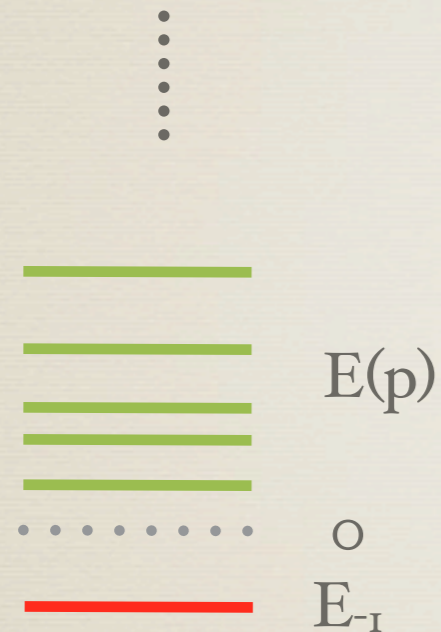
"back to back momentum"

nucleon-nucleon phase shifts

spin triplet

spin singlet
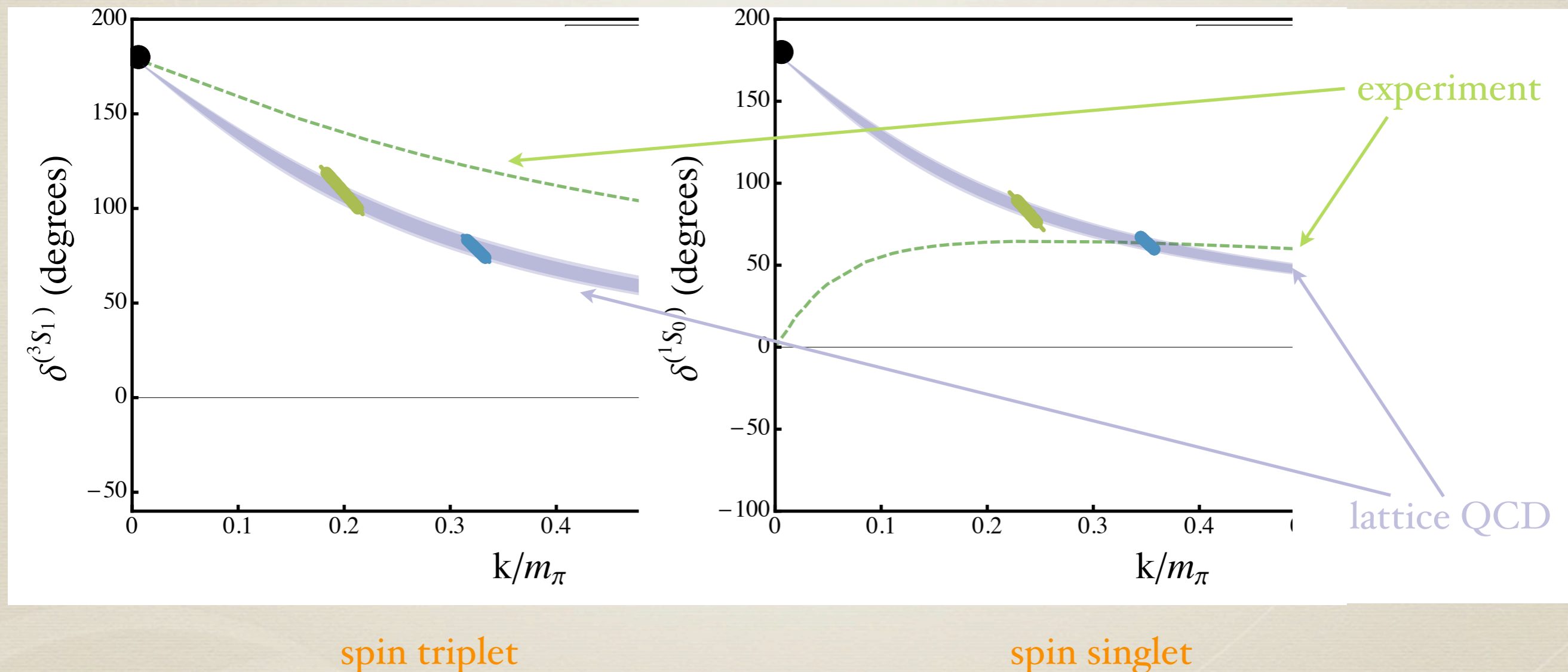
$M_\pi = 800 MeV$

degenerate up down and strange quarks

Conclusions

✳ Lattice QCD calculations are now addressing systems of few nucleons (baryon number larger than one)
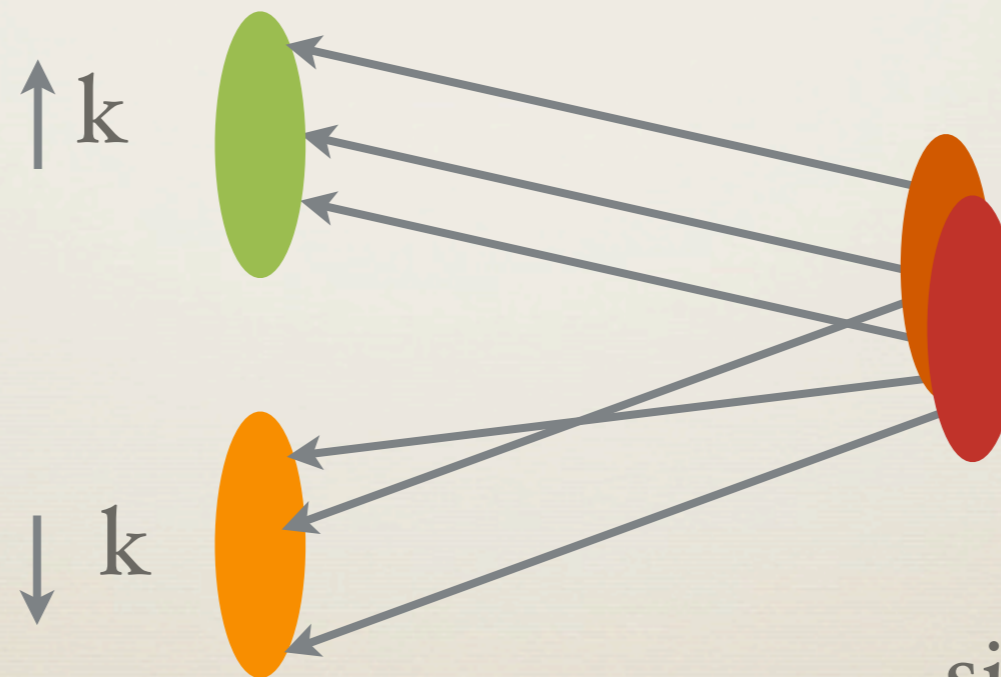
✳ New powerful supercomputers are key component to these efforts

✳ NPLQCD: Presented results for the spectrum of nuclei with A<5 and S>−3 at heavy quark masses (strange quark mass)

  ✳ As well as nucleon-nucleon phase shifts

✳ Significant challenges remain in performing calculations close to the physical point with controlled systematic errors

✳ With further improvements in methods and increase in available computational resources significant progress can be made

✳ A long term goal is for lattice calculations to provide input for determining the unknown parameters in an effective theory of nuclear forces which in turn it can be used to compute properties of large nuclei

THE END

Interpolating fields

Most general multi-baryon interpolating field

$$\bar{\mathcal{N}}^h = \sum_{\mathbf{a}} w_h^{a_1, a_2 \cdots a_{n_q}} \bar{q}(a_1)\bar{q}(a_2) \cdots \bar{q}(a_{n_q})$$

The indices a are composite including space, spin, color and flavor that can take N possible values

✳ The goal is to calculate the tensors w

✳ The tensors w are completely antisymmetric

✳ Number of terms in the sum are $$\frac{N!}{(N - n_q)!}$$

Nuclear interpolating fields

* Compute the hadronic weights

* Replace baryons by quark interpolating fields

* Perform Grassmann reductions

* Read off the reduced weights for the quark interpolating fields

* Computations done in: `algebra (C++)`

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{M_w} \tilde{W}_h^{(b_1, b_2 \cdots b_A)} \sum_{\mathbf{i}} \epsilon^{i_1, i_2, \cdots, i_A} \bar{B}(b_{i_1}) \bar{B}(b_{i_2}) \cdots \bar{B}(b_{i_A})$$

$$\bar{B}(b) = \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(a_1, a_2, a_3), k} \sum_{\mathbf{i}} \epsilon^{i_1, i_2, i_3} \bar{q}(a_{i_1}) \bar{q}(a_{i_2}) \bar{q}(a_{i_3})$$

$$\bar{\mathcal{N}}^h = \sum_{k=1}^{N_w} \tilde{w}_h^{(a_1, a_2 \cdots a_{n_q}), k} \sum_{\mathbf{i}} \epsilon^{i_1, i_2, \cdots, i_{n_q}} \bar{q}(a_{i_1}) \bar{q}(a_{i_2}) \cdots \bar{q}(a_{i_{n_q}})$$

Interpolating fields

Label	A	s	I	J^π	Local SU(3) irreps	int. field size
N	1	0	1/2	$1/2^+$	$\mathbf{8}$	9
Λ	1	-1	0	$1/2^+$	$\mathbf{8}$	12
Σ	1	-1	1	$1/2^+$	$\mathbf{8}$	9
Ξ	1	-2	1/2	$1/2^+$	$\mathbf{8}$	9
d	2	0	0	1^+	$\overline{\mathbf{10}}$	21
nn	2	0	1	0^+	$\mathbf{27}$	21
$n\Lambda$	2	-1	1/2	0^+	$\mathbf{27}$	96
$n\Lambda$	2	-1	1/2	1^+	$\mathbf{8}_A, \overline{\mathbf{10}}$	48, 75
$n\Sigma$	2	-1	3/2	0^+	$\mathbf{27}$	42
$n\Sigma$	2	-1	3/2	1^+	$\mathbf{10}$	27
$n\Xi$	2	-2	0	1^+	$\mathbf{8}_A$	96
$n\Xi$	2	-2	1	1^+	$\mathbf{8}_A, \mathbf{10}, \overline{\mathbf{10}}$	52,66,75
H	2	-2	0	0^+	$\mathbf{1}, \mathbf{27}$	90,132
^{3}H, ^{3}He	3	0	1/2	$1/2^+$	$\overline{\mathbf{35}}$	9
$^3_\Lambda$H$(1/2^+)$	3	-1	0	$1/2^+$	$\overline{\mathbf{35}}$	66
$^3_\Lambda$H$(3/2^+)$	3	-1	0	$3/2^+$	$\overline{\mathbf{10}}$	30
$^3_\Lambda$He,$^3_\Lambda\tilde{\text{H}}$, $nn\Lambda$	3	-1	1	$1/2^+$	$\mathbf{27}, \overline{\mathbf{35}}$	30,45
$^3_\Sigma$He	3	-1	1	$3/2^+$	$\mathbf{27}$	21
^{4}He	4	0	0	0^+	$\overline{\mathbf{28}}$	1
$^4_\Lambda$He, $^4_\Lambda$H	4	-1	1/2	0^+	$\overline{\mathbf{28}}$	6
$^4_{\Lambda\Lambda}$He	4	-2	1	0^+	$\mathbf{27}, \overline{\mathbf{28}}$	15, 18
$\Lambda\Xi^0 pnn$	5	-3	0	$3/2^+$	$\overline{\mathbf{10}} + ...$	1

Interpolating fields

Label	A	s	I	J^π	Local SU(3) irreps	int. field size
N	1	0	1/2	$1/2^+$	$\mathbf{8}$	9
Λ	1	-1	0	$1/2^+$	$\mathbf{8}$	12
Σ	1	-1	1	$1/2^+$	$\mathbf{8}$	9
Ξ	1	-2	1/2	$1/2^+$	$\mathbf{8}$	9
d	2	0	0	1^+	$\overline{\mathbf{10}}$	21
nn	2	0	1	0^+	$\mathbf{27}$	21
$n\Lambda$	2	-1	1/2	0^+	$\mathbf{27}$	96
$n\Lambda$	2	-1	1/2	1^+	$\mathbf{8}_A, \overline{\mathbf{10}}$	48, 75
$n\Sigma$	2	-1	3/2	0^+	$\mathbf{27}$	42
$n\Sigma$	2	-1	3/2	1^+	$\mathbf{10}$	27
$n\Xi$	2	-2	0	1^+	$\mathbf{8}_A$	96
$n\Xi$	2	-2	1	1^+	$\mathbf{8}_A, \mathbf{10}, \overline{\mathbf{10}}$	52,66,75
H	2	-2	0	0^+	$\mathbf{1}, \mathbf{27}$	90,132
^{3}H, ^{3}He	3	0	1/2	$1/2^+$	$\overline{\mathbf{35}}$	9
$^3_\Lambda$H$(1/2^+)$	3	-1	0	$1/2^+$	$\overline{\mathbf{35}}$	66
$^3_\Lambda$H$(3/2^+)$	3	-1	0	$3/2^+$	$\overline{\mathbf{10}}$	30
$^3_\Lambda$He,$^3_\Lambda\tilde{\text{H}}$, $nn\Lambda$	3	-1	1	$1/2^+$	$\mathbf{27}, \overline{\mathbf{35}}$	30,45
$^3_\Sigma$He	3	-1	1	$3/2^+$	$\mathbf{27}$	21
^{4}He	4	0	0	0^+	$\overline{\mathbf{28}}$	1
$^4_\Lambda$He, $^4_\Lambda$H	4	-1	1/2	0^+	$\overline{\mathbf{28}}$	6
$^4_{\Lambda\Lambda}$He	4	-2	1	0^+	$\mathbf{27}, \overline{\mathbf{28}}$	15, 18
$\Lambda\Xi^0 pnn$	5	-3	0	$3/2^+$	$\overline{\mathbf{10}} + ...$	1

Wick contraction methods

Quarks to Quarks

Quarks to Hadrons

$\vec{P}$

single point source

single point source

M terms   N terms

$\vec{p_A}$

$\vec{p_2}$

$\vec{p_1}$

N terms   M terms
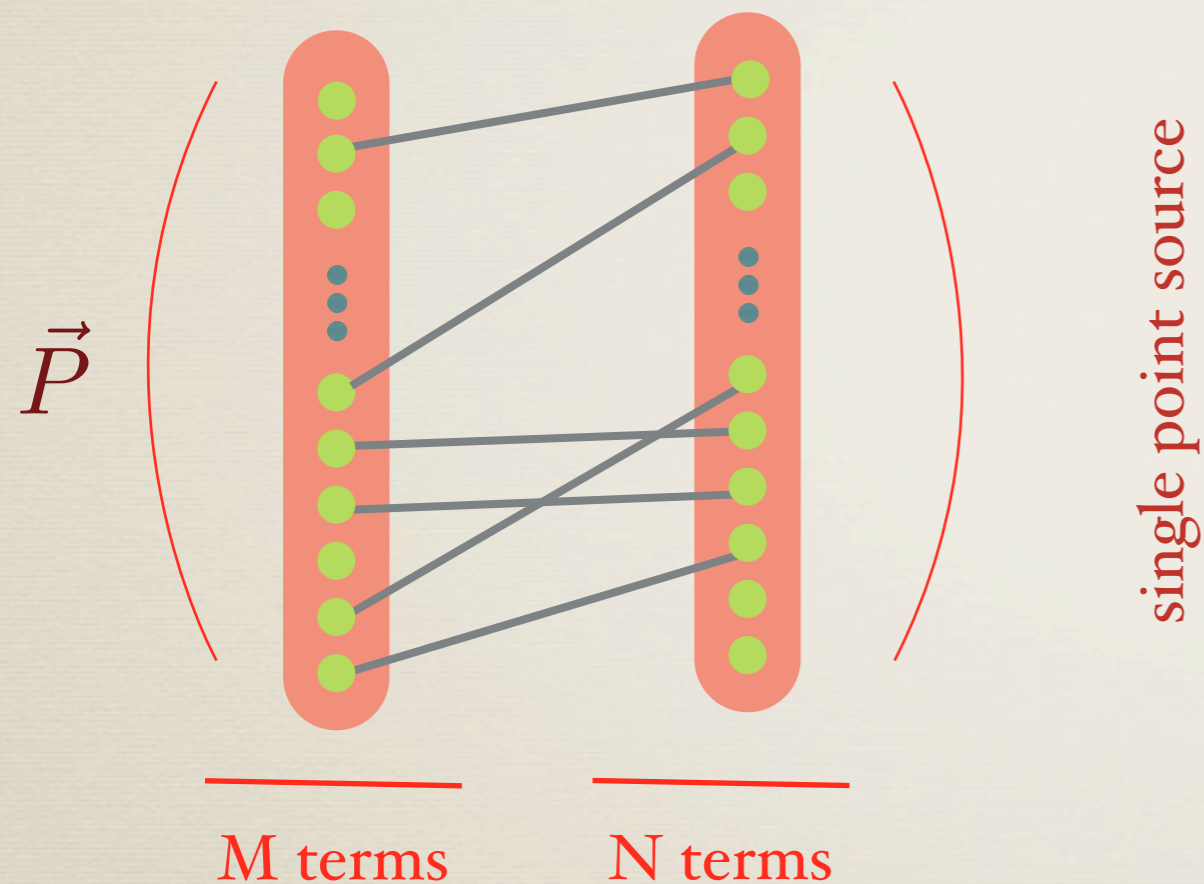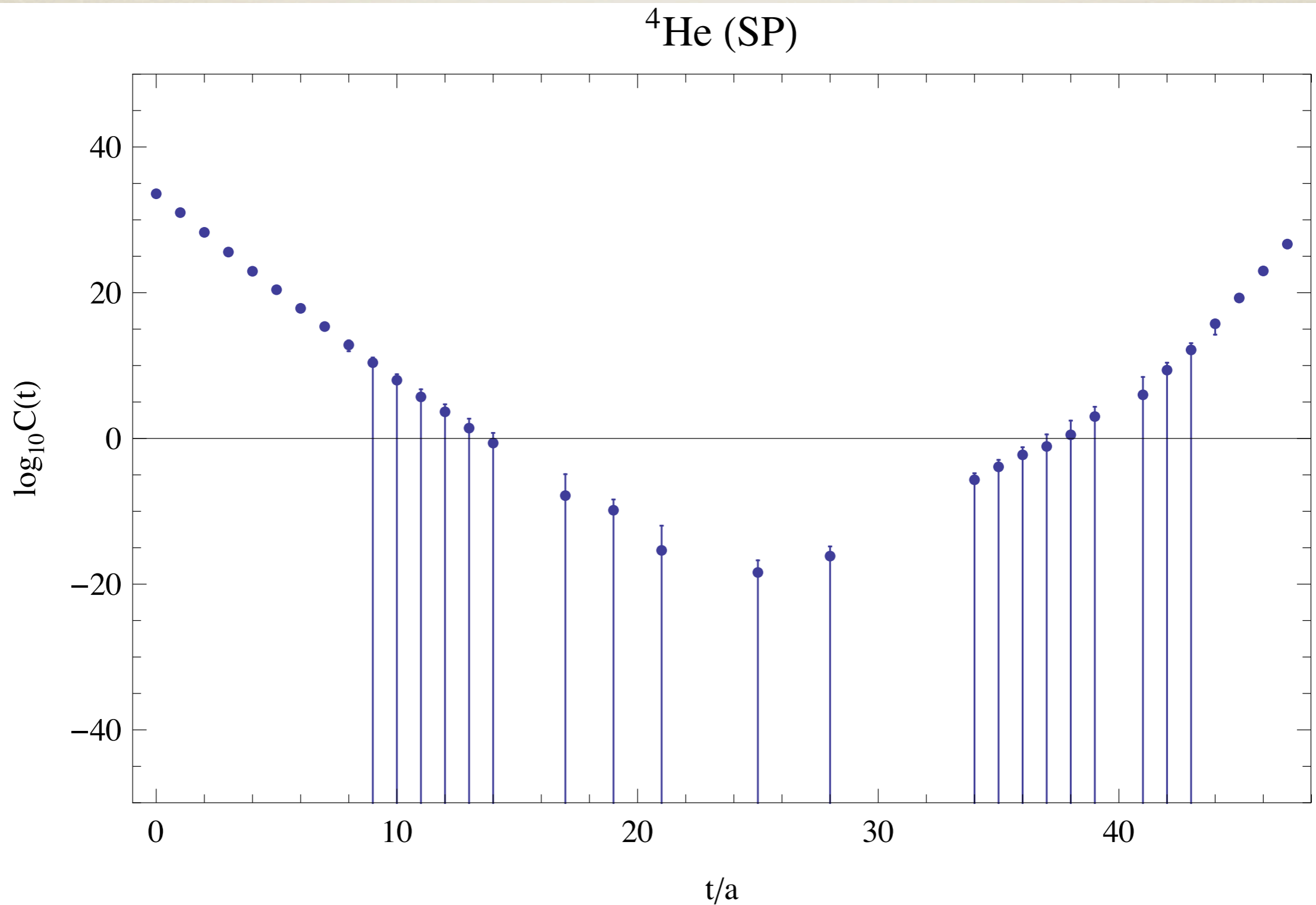
Naive Cost: $\quad n_u! n_d! n_s! \times NM$

Actual Cost: $\quad n_u^3 n_d^3 n_s^3 \times MN$
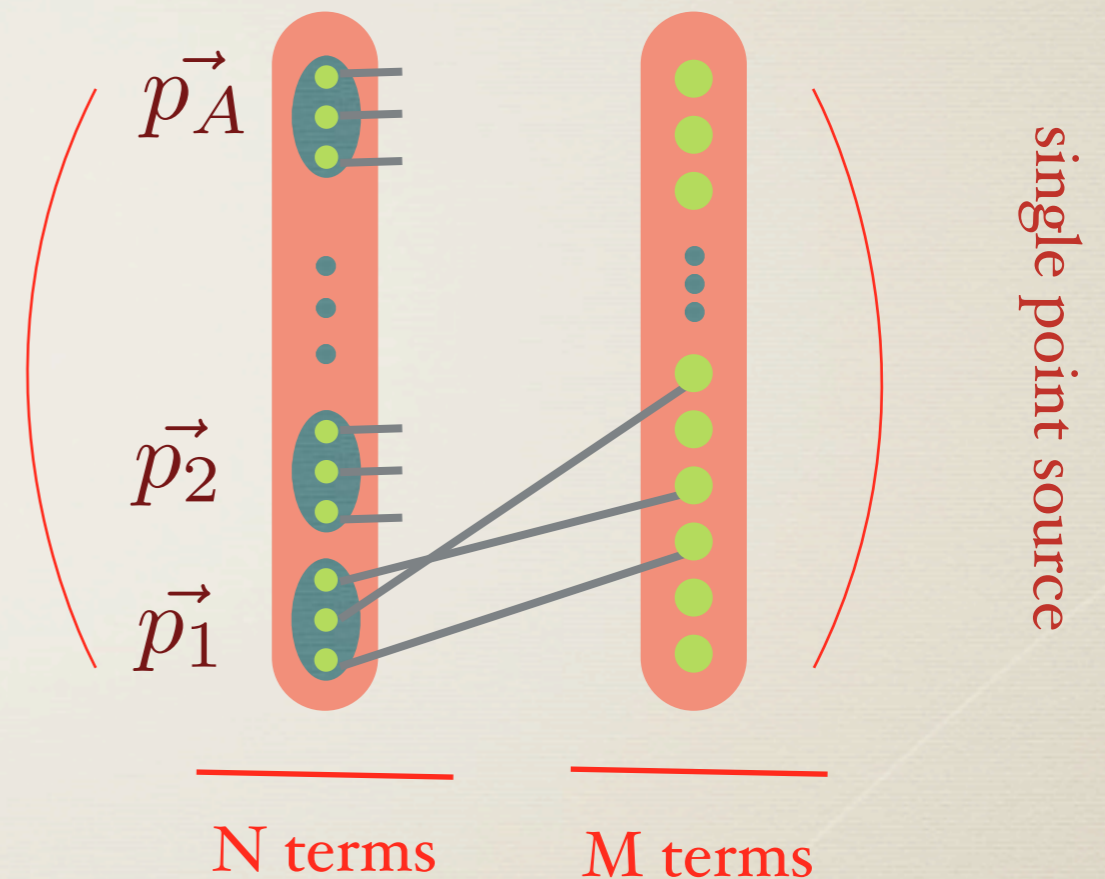
Cost: $\quad M \cdot N \dfrac{n_u! n_d! n_s!}{2^{(A - n_{\Sigma^0} - n_\Lambda)}}$

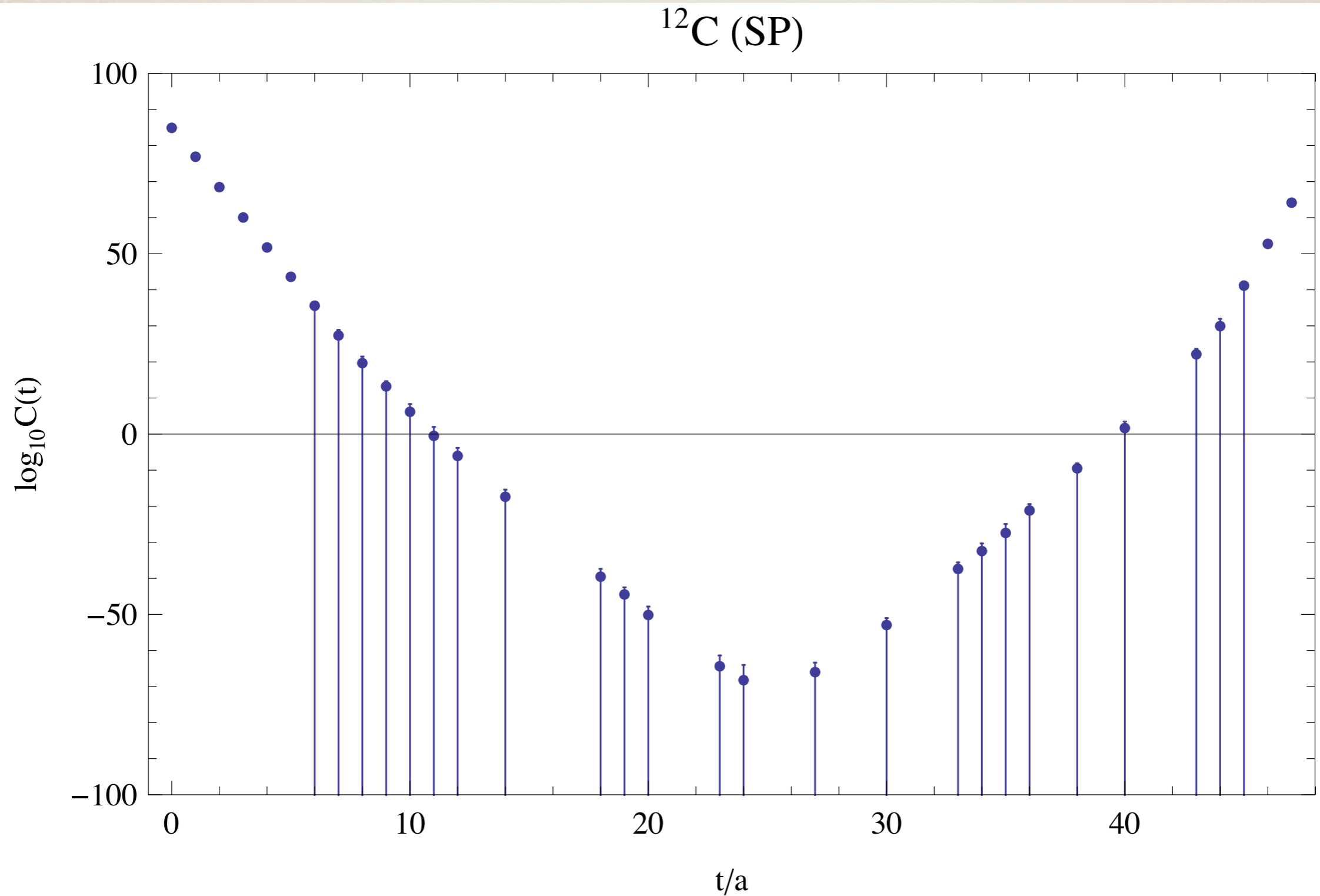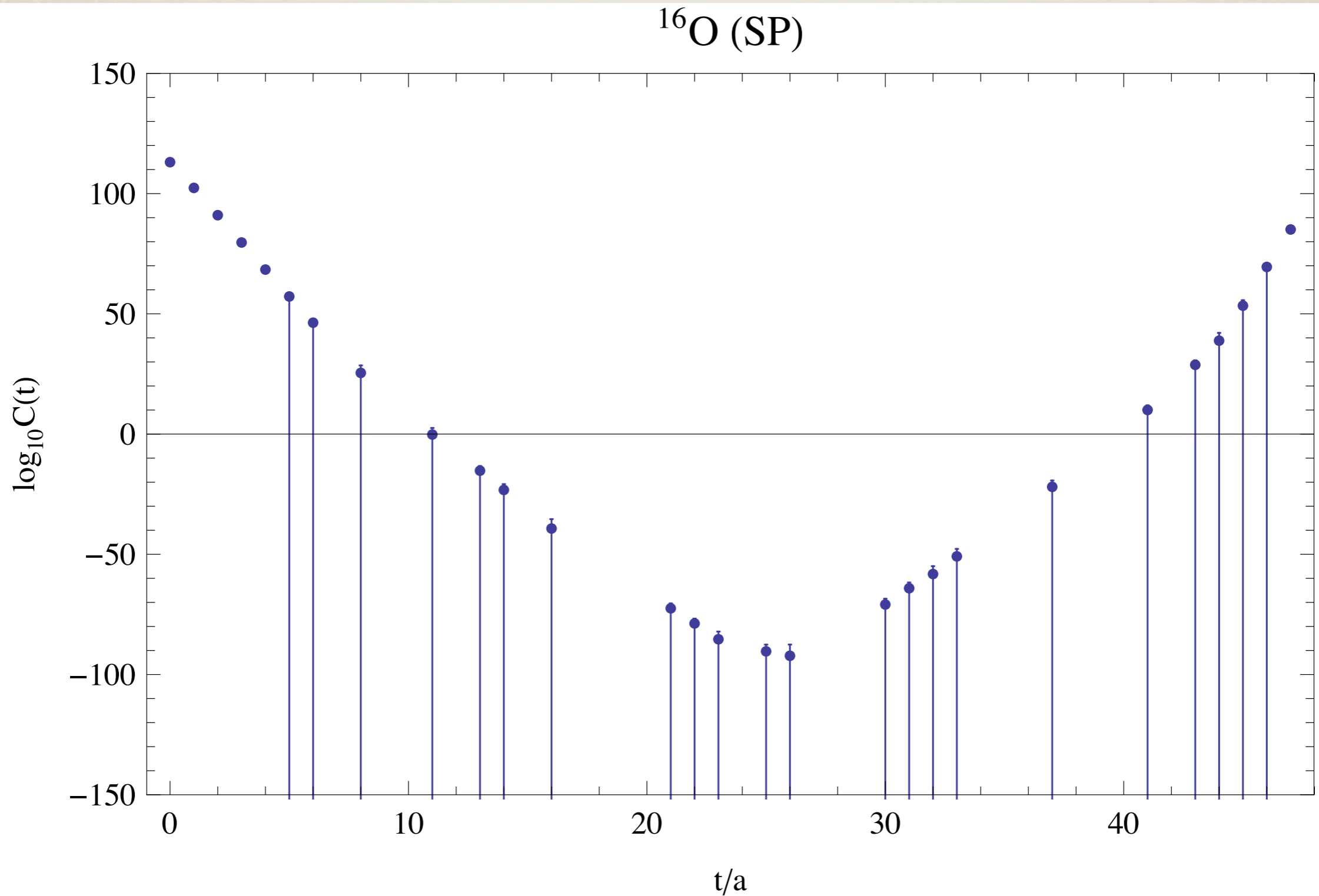# Correlators for large nucleii
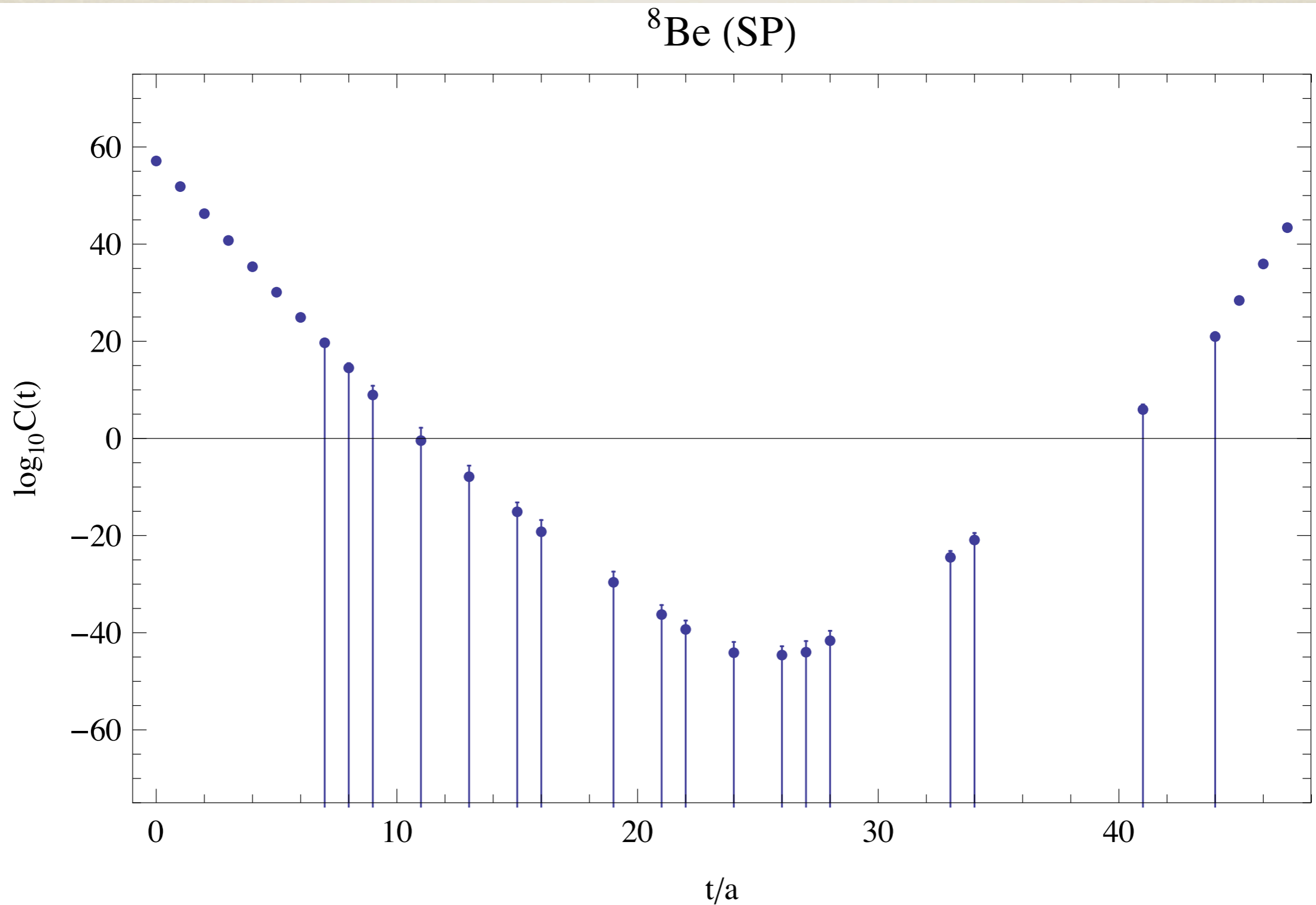
^{4}He (SP)

Correlators for large nucleii

^{8}Be (SP)

Correlators for large nucleii

^{12}C (SP)

Correlators for large nucleii

^{16}O (SP)
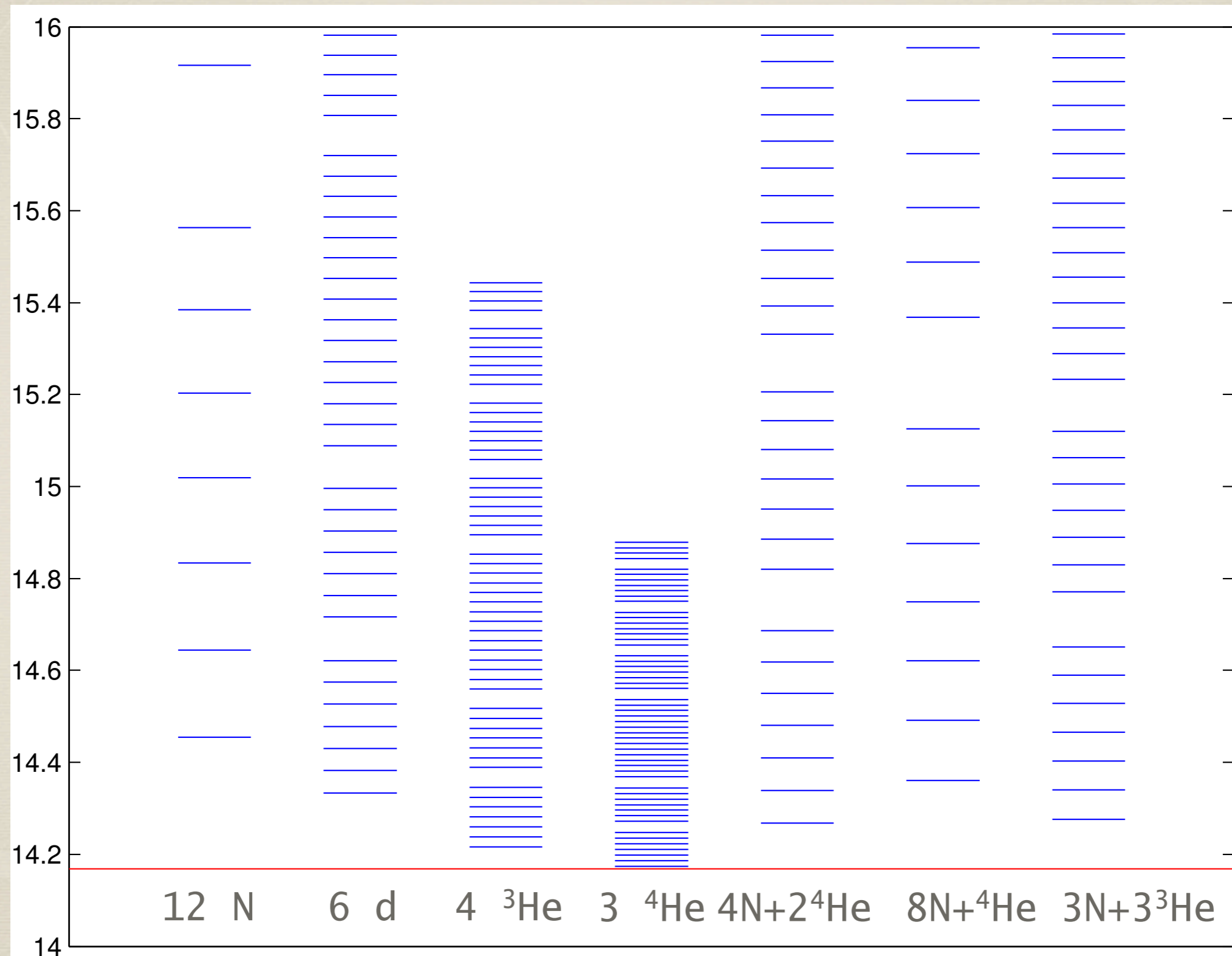
Correlators for large nucleii

^{28}Si (SP)
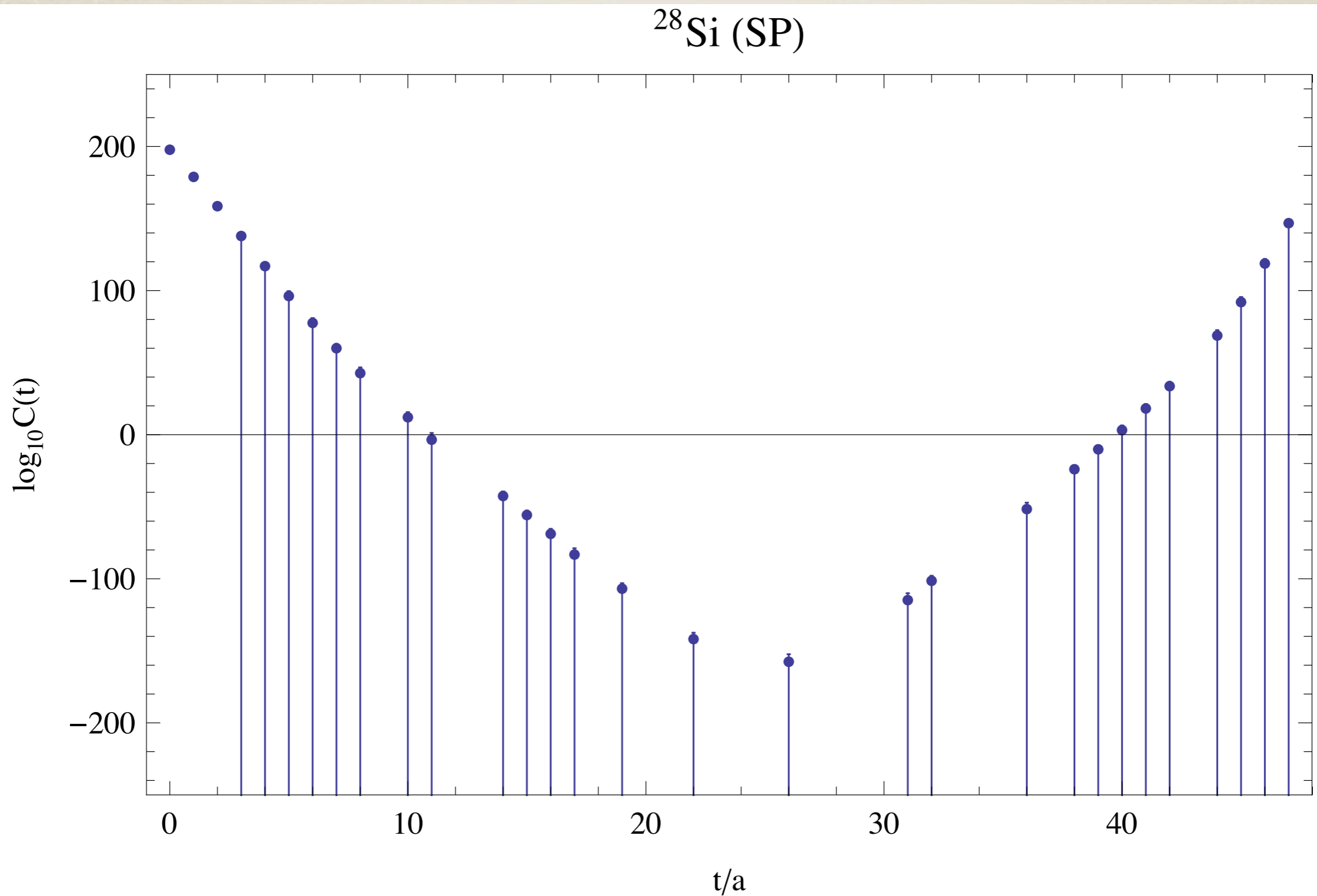
Expected Carbon spectrum in the 32^3 box

Expected Carbon spectrum in the 32³ box